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Four Essays on Sequential Monte Carlo and Quasi-Monte Carlo Methods

GERBER Mathieu

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Four Essays on Sequential Monte Carlo and Quasi-Monte Carlo Methods

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pour l'obtention du grade de
Docteur en Sciences Economiques, mention « Economie politique »

par

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La thèse est intitulée :

FOUR ESSAYS ON SEQUENTIAL MONTE CARLO AND QUASI-MONTE CARLO METHODS

Lausanne, le 25 novembre 2014

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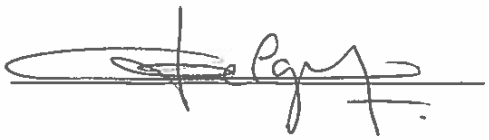
Signature :  Date : 24 Novembre 2014

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Contents

Introduction

Sequential Monte Carlo algorithms (or particle filtering) were introduced by Gordon et al. (1993) to carry out sequential inference in state-space models. State-space models, popular in many fields such as Economics, Engineering and Neuroscience, are used for extracting information about a hidden Markov process $(\mathbf{x}_t)_{t\geq 0}$ of interest from a set of $T+1$ observations $\mathbf{y}_{0:T} = (\mathbf{y}_0, \ldots, \mathbf{y}_T)$. In practice, this typically translates to the estimation of $p(\mathbf{x}_t|\mathbf{y}_{0:t})$, the distribution of $\mathbf{x}_t$ given the data $\mathbf{y}_{0:t}$, which is called the *filtering* distribution. Often, state-space models are indexed by a vector of parameters that should be learnt from the likelihood function of the data, $p(\mathbf{y}_{0:T})$. However, except in very specific scenarios, it is well known that the filtering distributions and the likelihood function are intractable and therefore approximation techniques have to be used both for parameter and state estimation.

The basic idea of particle filtering, as introduced by Gordon et al. (1993), is to first construct a Monte Carlo approximation $\pi_0^N(\mathrm{d}\mathbf{x}_0) = \sum_{n=1}^N W_0^n \delta_{\mathbf{x}_0^n}(\mathrm{d}\mathbf{x}_0)$ of the filtering distribution at time $t=0$, $\pi_0(\mathrm{d}\mathbf{x}_0) := p(\mathbf{x}_0|\mathbf{y}_0)\mathrm{d}\mathbf{x}_0$, where $\{\mathbf{x}_0^n\}_{n=1}^N$ is a set of simulations (called *particles*) from a proposal distribution $q_0(\mathrm{d}\mathbf{x}_0)$ while $\{W_0^n\}_{n=1}^N$ are the corresponding (self normalized) importance weights. Then, using successions of resampling and mutation steps, sequential Monte Carlo (SMC) algorithms construct iteratively an approximation $\pi_t^N(\mathrm{d}\mathbf{x}_t) = \sum_{n=1}^N W_t^n \delta_{\mathbf{x}_t^n}(\mathrm{d}\mathbf{x}_t)$ of the filtering distribution at time $t \geq 1$, $\pi_t(\mathrm{d}\mathbf{x}_t) := p(\mathbf{x}_t|\mathbf{y}_{0:t})\mathrm{d}\mathbf{x}_t$, where, again, $\{\mathbf{x}_t^n\}_{n=1}^N$ are simulations from a proposal distribution and $\{W_t^n\}_{n=1}^N$ are the corresponding weights.

Since the seminal paper of Gordon et al. (1993) the development of particle filtering has taken several directions. In particular, there has been a lot of works on SMC error rates which, informally, can be written at iteration t of SMC as $C_t N^{-1/2}$, where C_t is some function of t. For instance, Del Moral (2004) provides conditions for the error rate to be bounded uniformly in time, i.e. to have $C_t \leq C$, while other authors have worked on the reduction of C_t through more efficient algorithmic designs, such as better proposal kernels or resampling schemes (see Douc and Cappé, 2005, for a review and a comparison of resampling algorithms). The research on SMC methods has been boosted further by the paper of Andrieu et al. (2010) which shows that particle filters can be used as a proposal mechanism within Markov Chain Monte Carlo (MCMC) methods, leading to the so-called particle MCMC (PMCMC) algorithms. For instance, because of the high running time of PMCMC algorithms,

which require to run a particle filter at each iteration of the Markov chain, several recent papers are devoted to the construction of parallelized (and hence faster) SMC algorithms (see e.g. Vergé et al., 2013; Murray et al., 2014; Paige et al., 2014).

In the first three chapters of this thesis we contribute to the development of sequential estimation methods for state-space models in a direction which has been almost unexplored until now, namely the introduction of quasi-Monte Carlo (QMC) ideas inside the SMC framework; that is, to build a sequential quasi-Monte Carlo (SQMC) algorithm. Informally, a QMC point set is a deterministic set of points that looks "more uniform" than a random sample of uniform variates, while randomized QMC (RQMC) point sets combine the advantage of random sampling and QMC strategies, namely they both spread evenly over unit hypercubes and are such that marginally every point is uniformly distributed. As illustrated in the following quote, one can expect better convergence properties of quadrature rules which rely on QMC point sets that those relying on (pseudo-)random numbers:

> On s'est aperu que le rendement, assez faible d'ailleurs, réclamé par la méthode de Monte Carlo peut être dépassé de loin si, au lieu de former la moyenne de l'intégrande sur un ensemble choisi au petit bonheur, on le fait sur un ensemble déterminé d'une façon judicieuse. (Zaremba, 1972)

Based on this idea, the first three chapters of this thesis therefore focuses on the second factor $N^{-1/2}$ of the SMC error rate, i.e. we want the error rate to converge quicker relative to N than the standard Monte Carlo rate $N^{-1/2}$.

The SQMC algorithm, developed in Chapter 1, is related to, and may be seen as an extension of, the array-RQMC algorithm of L'Ecuyer et al. (2006). With a complexity of $\mathcal{O}(N \log N)$, where we recall that N is the number of simulations at each iteration, SQMC is slightly slower than SMC but its error rate is smaller than the Monte Carlo rate $\mathcal{O}_P(N^{-1/2})$. The only requirement to implement SQMC is the ability to write in the mutation step the simulation of particle $\mathbf{x}_t^n$ given $\mathbf{x}_{t-1}^n$ as a deterministic function of $\mathbf{x}_{t-1}^n$ and a fixed number of uniform variates. Since SQMC provides an unbiased likelihood evaluation, it may serve as an efficient alternative to SMC within a PMCMC algorithm.

So far, we have presented SMC as a way to estimate the likelihood function and the filtering distributions in state-space models. However, we may also be interested in computing $p(\mathbf{x}_{0:T}|\mathbf{y}_{0:T})$, that is, the *smoothing* distribution. To that purpose we propose and analyse in Chapter 2 quasi-Monte Carlo smoothing algorithms. In particular, we study QMC versions of forward-backward smoothing (Doucet et al., 2000; Godsill et al., 2004) and of two filter smoothing (Briers et al., 2010). As shown in a numerical study, these QMC smoothing methods outperform their Monte Carlo counterpart. Since the complexity of these algorithms is $\mathcal{O}(N^2)$, even small gains (in term of mean square errors) for QMC techniques translate into important savings in term of running time.

As we will argue through Chapter 1, using nested scrambled (t, s)-sequences in base $b \geq 2$ (Owen, 1995) as inputs of SQMC is the right choice for the randomized version of the algorithm. In particular, all the results on stochastic bounds hold for this particular construction of RQMC point sets, which is known to have several nice properties when used to solve "simple" integration problems. To be more specific, let $I(\varphi) = \int_{[0,1)^s} \varphi(\mathbf{x}) \mathrm{d}\mathbf{x}$ for a function $\varphi \in L_2[0,1)^s$. Then, the estimate $N^{-1} \sum_{n=0}^{N-1} \varphi(\mathbf{x}^n)$ of $I(\varphi)$ has an error of size $o_P(N^{-1/2})$ when $\{\mathbf{x}^n\}_{n=1}^N$ are the first N points of a scrambled (t, s)-sequence in base $b \geq 2$ (Owen, 1995, 1997a,b, 1998). However, one limitation of this result is that it only applies for $N = \lambda b^m$, $1 \leq \lambda < b$, this restriction arising because (t, s)-sequences in base b are characterized by their equidistribution properties on sets of b^m consecutive points, $m \geq t$. From a practical point of view, this means that a variance reduction can only be obtained at the price of a sharply increasing running time, which may reduce the attractiveness of scrambled net integration methods when one is interested e.g. to reach a given level of precision at the lowest computational effort. Going back to SQMC, this for instance happens when SQMC is used as a proposal inside a Metropolis-Hastings algorithm (Pitt et al., 2012; Doucet et al., 2013; Sherlock et al., 2013).

In Chapter 3 we show that this constraint on N is in fact not necessary for methods based on scrambled nets to outperform plain Monte Carlo. In particular, we show that, both for unweighted quadrature rules and for SQMC, using scrambled nets of size N as inputs yields an error of size $o_P(N^{-1/2})$ regardless the choice of N. Approximation errors of these integration methods are compared in a numerical study which shows that for unweighted quadrature rules we can relax the constraint $N = \lambda b^m$ without any loss of efficiency when the integrand is discontinuous. Since SQMC involves integration of discontinuous functions this suggests that the behaviour of the approximation error should not be very sensitive to the choice of N. This point is illustrated in a simulation study based on two univariate state-space models and we argue that for multivariate models it is very unlikely to expect any gain of imposing $N = \lambda b^m$.

If SMC was initially introduced to carry out inference in state-space models, the methodology has been afterwards extended to non dynamic models by Neal (2001); Chopin (2002); Del Moral et al. (2006). In that case, SMC is applied on the sequence of distribution $\{\pi_t\}_{t=0}^T$ where π_T is the distribution we want to sample from and $\{\pi_t\}_{t=0}^{T-1}$ is a user defined sequence of auxiliary distributions. Such a simulations technique is now widely used in Bayesian parameter inference which often requires to sample from complicated posterior distributions, and is known to outperform MCMC methods in some cases.

In the last chapter of this thesis we illustrate the usefulness of SMC in static models by applying this sampling strategy for Bayesian parameter inference in extended-skew normal distributions. The extended skew-normal distribution, which belongs to the class of skew-elliptical distributions, allows for accommodating with addi-

tional parameters raw data which are skewed and heavy tailed while being tractable and parsimonious, and having at least three appealing statistical properties, namely closure under conditioning, affine transformations, and marginalization. In the last chapter of this thesis, we propose a Bayesian estimation approach based on a tempered sequential Monte Carlo algorithm. The practical implementation of each step of the algorithm is discussed and the elicitation of the prior distributions takes into consideration some unusual behaviour of the likelihood function and the corresponding Fisher information matrix. Using Monte Carlo simulations, we provide strong evidence regarding the statistical performances of the SMC sampler as well as some new insights regarding the parametrizations (latent representation and convolution representation) of the extended skew-normal distributions. A generalization to the extended skew-normal sample selection model is also presented. Finally we proceed with the analysis of two real datasets which show the usefulness of this family of distribution in practical scenarios.

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Chapter 1

Sequential Quasi-Monte Carlo

Joint work with Nicolas Chopin (ENSAE/CREST)

Abstract

We derive and study SQMC (Sequential Quasi-Monte Carlo), a class of algorithms obtained by introducing QMC point sets in particle filtering. SQMC is related to, and may be seen as an extension of, the array-RQMC algorithm of L'Ecuyer et al. (2006). The complexity of SQMC is $\mathcal{O}(N \log N)$, where N is the number of simulations at each iteration, and its error rate is smaller than the Monte Carlo rate $\mathcal{O}_P(N^{-1/2})$. The only requirement to implement SQMC is the ability to write the simulation of particle $\mathbf{x}_t^n$ given $\mathbf{x}_{t-1}^n$ as a deterministic function of $\mathbf{x}_{t-1}^n$ and a fixed number of uniform variates. We show that SQMC is amenable to the same extensions as standard SMC, such as forward smoothing, backward smoothing, unbiased likelihood evaluation, and so on. In particular, SQMC may replace SMC within a PMCMC (particle Markov chain Monte Carlo) algorithm. We establish several convergence results. We provide numerical evidence that SQMC may significantly outperform SMC in practical scenarios.

Keywords: Array-RQMC; Low discrepancy; Particle filtering; Quasi-Monte Carlo; Randomized Quasi-Monte Carlo; Sequential Monte Carlo

1.1 Introduction

Sequential Monte Carlo (SMC, also known as particle filtering) is a class of algorithms for computing recursively Monte Carlo approximations of a sequence of distributions $\pi_t(\mathrm{d}\mathbf{x}_t)$, $t \in 0{:}T$, $0{:}T = \{0, \ldots, T\}$. The initial motivation of SMC was the filtering of state-space models (also known as hidden Markov models); that is, given a latent Markov process $(\mathbf{x}_t)$, observed imperfectly as e.g. $\mathbf{y}_t = f(\mathbf{x}_t) + \epsilon_t$, recover at every time t the distribution of $\mathbf{x}_t$ given the data $\mathbf{y}_{0:t} = (\mathbf{y}_0, \ldots, \mathbf{y}_t)$.

SMC's popularity stems from the fact it is the only realistic approach for filtering and related problems outside very specific cases (such as the linear Gaussian model). Recent research has further increased interest in SMC, especially in Statistics, in at least two directions. First, several papers (Neal, 2001; Chopin, 2002; Del Moral et al., 2006) have extended SMC to non-sequential problems; that is, to sample from distribution π, one applies SMC to some artificial sequence π_t that ends up at $\pi_T = \pi$. In certain cases, such an approach outperforms MCMC (Markov chain Monte Carlo) significantly. Second, the seminal paper of Andrieu et al. (2010) established that SMC may be used as a proposal mechanism within MCMC, leading to so called PMCMC (particle MCMC) algorithms. While not restricted to such problems, PMCMC is the only possible approach for inference in state-space models such that the transition kernel of $(\mathbf{x}_t)$ may be sampled from, but does not admit a tractable density. Excitement about PMCMC is evidenced by the 30 papers or so that have appeared in the last two years on possible applications and extensions.

Informally, the error rate of SMC at iteration t is $C_t N^{-1/2}$, where C_t is some function of t. There has been a lot of work on SMC error rates (e.g. Del Moral, 2004), but it seems fair to say that most of it has focussed on the first factor C_t; that is, whether to establish that the error rate is bounded uniformly in time, $C_t \leq C$, or to reduce C_t through more efficient algorithmic designs, such as better proposal kernels or resampling schemes.

In this work, we focus on the second factor $N^{-1/2}$, i.e. we want the error rate to converge quicker relative to N than the standard Monte Carlo rate $N^{-1/2}$. To do so, we adapt to the SMC context ideas borrowed from QMC (Quasi-Monte Carlo); that is, the idea of replacing random numbers by low discrepancy point sets.

The following subsections contain very brief introductions to SMC and QMC, with an exclusive focus on the concepts that are essential to follow this work. For a more extensive presentation of SMC, the reader is referred to the books of Doucet et al. (2001), Del Moral (2004) and Cappé et al. (2005), while for QMC and RQMC, see Chapter 5 of Glasserman (2004), Chapters 5 and 6 of Lemieux (2009), and Dick and Pillichshammer (2010).

1.1.1 Introduction to SMC

As already mentioned, the initial motivation of SMC is the sequential analysis of state-space models; that, is models for a Markov chain $(\mathbf{x}_t)$ in $\mathcal{X} \subseteq \mathbb{R}^d$,

$$\mathbf{x}_0 \sim f_0^X(\mathbf{x}_0), \quad \mathbf{x}_t|\mathbf{x}_{t-1} \sim f^X(\mathbf{x}_t|\mathbf{x}_{t-1}),$$

which is observed only indirectly through some $\mathbf{y}_t$, with density $\mathbf{y}_t|\mathbf{x}_t \sim f^Y(\mathbf{y}_t|\mathbf{x}_t)$.

This kind of model arises in many areas of science: in tracking for instance, $\mathbf{x}_t$ may be the position of a ship (in two dimensions) or a plane (in three dimensions), and $\mathbf{y}_t$ may be a noisy angular observation (radar). In Ecology, $\mathbf{x}_t$ would be the size of a population of bats in a cave, and $\mathbf{y}_t$ would be $\mathbf{x}_t$ plus noise. And so on.

The most standard inferential task for such models is that of *filtering*; that is, to recover iteratively in time t, $p(\mathbf{x}_t|\mathbf{y}_{0:t})$, the distribution of $\mathbf{x}_t$, given the data collected up time t, $\mathbf{y}_{0:t} = (\mathbf{y}_0, \ldots, \mathbf{y}_t)$. One may also be interested in smoothing, $p(\mathbf{x}_{0:t}|\mathbf{y}_{0:t})$, or likelihood evaluation, $p(\mathbf{y}_{0:t})$, notably when the model depends on a fixed parameter θ which should be learnt from the data.

A simple Monte Carlo approach to filtering is sequential importance sampling: choose an initial distribution $m_0(\mathrm{d}\mathbf{x}_0)$, a sequence of Markov kernels $m_t(\mathbf{x}_{t-1}, \mathrm{d}\mathbf{x}_t)$, $t \geq 1$, then simulate N times iteratively from these m_t's, $\mathbf{x}_0^n \sim m_0(\mathrm{d}\mathbf{x}_0)$, $\mathbf{x}_t^n|\mathbf{x}_{t-1}^n \sim m_t(\mathbf{x}_{t-1}^n, \mathrm{d}\mathbf{x}_t)$, and reweight 'particle' (simulation) $\mathbf{x}_t^n$ as follows: $w_0^n = G_0(\mathbf{x}_0^n)$, $w_t^n = w_{t-1}^n \times G_t(\mathbf{x}_{t-1}^n, \mathbf{x}_t^n)$, where the weight functions G_t are defined as

$$G_0(\mathbf{x}_0) = \frac{f^Y(\mathbf{y}_0|\mathbf{x}_0) f_0^X(\mathbf{x}_0)}{m_0(\mathbf{x}_0)}, \quad G_t(\mathbf{x}_{t-1}, \mathbf{x}_t) = \frac{f^Y(\mathbf{y}_t|\mathbf{x}_t) f^X(\mathbf{x}_t|\mathbf{x}_{t-1})}{m_t(\mathbf{x}_t|\mathbf{x}_{t-1})}, \tag{1.1}$$

and $m_t(\mathbf{x}_t|\mathbf{x}_{t-1})$ in the denominator denotes the conditional probability density associated to kernel $m_t(\mathbf{x}_{t-1}, \mathrm{d}\mathbf{x}_t)$. Then it is easy to check that the weighted average $\sum_{n=1}^N w_t^n \varphi(\mathbf{x}_t^n) / \sum_{n=1}^N w_t^n$ is a consistent estimate of the filtering expectation $\mathbb{E}[\varphi(\mathbf{x}_t)|\mathbf{y}_{0:t}]$, as $N \to +\infty$. However, it is well known that, even for carefully chosen proposal densities m_t, sequential importance sampling quickly degenerates: as time progresses, more and more particles get a negligible weight.

Surprisingly, there is a simple solution to this degeneracy problem: one may *resample* the particles; that is, draw N times with replacement from the set of particles, with probabilities proportional to the weights w_t^n. In this way, particles with low weight gets quickly discarded, while particles with large weight may get many children at the following iteration. Empirically, the impact of resampling is dramatic: the variance of filtering estimates typically remains stable over time, while without resampling it diverges exponentially fast.

The idea of using resampling may be traced back to Gordon et al. (1993), and has initiated the whole field of particle filtering. See Algorithm 1.1 for a summary of a basic PF (particle filter). The price to pay for introducing resampling is that it creates non-trivial dependencies between the particles, which complicates the formal study of such algorithms. In particular, establishing convergence (as $N \to +\infty$) is non-trivial, although the error rate of SMC is known to be $\mathcal{O}_P(N^{-1/2})$; see e.g. the central limit theorems of Del Moral and Guionnet (1999), Chopin (2004) and Künsch (2005). We shall see that it is also the resampling step that makes the introduction of Quasi-Monte Carlo into SMC non-trivial.

The complexity of SMC is $\mathcal{O}(N)$. In particular, to implement the resampling step in $\mathcal{O}(N)$ time (Step (a) at times $t \geq 1$ in Algorithm 1.1), one proceeds as follows: (a) generate $u^{1:N} = \mathrm{sort}(v^{1:N})$, where the v^n are independent uniform variates (see p.214 of Devroye, 1986, for a well-known algorithm to generate $u^{1:N}$ directly in $\mathcal{O}(N)$ time, without any sorting); and (b) use the inverse transform method for discrete distributions, recalled in Algorithm 1.2. We will re-use Algorithm 1.2 in SQMC.

Algorithm 1.1 Basic particle filter

At time $t = 0$,

(a) Generate $\mathbf{x}_0^n \sim m_0(\mathrm{d}\mathbf{x}_0)$ for all $n \in 1{:}N$.

(b) Compute $w_0^n = G_0(\mathbf{x}_0^n)$ and $W_0^n = w_0^n / \sum_{m=1}^N w_0^m$ for all $n \in 1{:}N$.

From time $t = 1$ to time T,

(a) Generate $a_{t-1}^n \sim \mathcal{M}(W_{t-1}^{1:N})$ for all $n \in 1{:}N$, the multinomial distribution that produces outcome m with probability W_{t-1}^m. See Algorithm 1.2.

(b) Generate $\mathbf{x}_t^n \sim m_t(\mathbf{x}_{t-1}^{a_{t-1}^n}, \mathrm{d}\mathbf{x}_t)$ for all $n \in 1{:}N$.

(c) Compute $w_t^n = G_t(\mathbf{x}_{t-1}^{a_{t-1}^n}, \mathbf{x}_t^n)$, and $W_t^n = w_t^n / \sum_{m=1}^N w_t^m$ for all $n \in 1{:}N$.

Algorithm 1.2 Resampling Algorithm (inverse transform method)

Input: $u^{1:N}$ (such that $0 \leq u^1 \leq \ldots \leq u^N \leq 1$), $W^{1:N}$ (normalised weights)
Output: $a^{1:N}$ (labels in $1:N$)

```
s ← W^1, m ← 1
for n = 1 → N do
    while s < u^n do
        m ← m + 1
        s ← s + W^m
    end while
    a^n ← m
end for
```

1.1.2 Introduction to QMC

QMC (Quasi-Monte Carlo) is generally presented as a way to perform integration with respect to the (semi-closed) hypercube of dimension d:

$$\frac{1}{N}\sum_{n=1}^{N}\varphi(\mathbf{u}^n) \approx \int_{[0,1)^d}\varphi(\mathbf{u})\,\mathrm{d}\mathbf{u}$$

where the N vectors $\mathbf{u}^n \in [0,1)^d$ must be chosen so as to have "low discrepancy", that is, informally, to be spread evenly over $[0,1)^d$. (We respect the standard convention in the QMC literature to work with space $[0,1)^d$, rather than $[0,1]^d$, as it turns out to be technically more convenient.)

Formally, the general notion of discrepancy is defined as

$$D(\mathbf{u}^{1:N};\mathcal{A}) = \sup_{A\in\mathcal{A}}\left|\frac{1}{N}\sum_{n=1}^{N}\mathbb{1}\left(\mathbf{u}^n\in A\right) - \lambda_d(A)\right|$$

where $\lambda_d(A)$ is the volume (Lebesgue measure on $\mathbb{R}^d$) of A, and $\mathcal{A}$ is a set of measurable sets. Two discrepancies are particularly useful in this work: the extreme discrepancy,

$$D(\mathbf{u}^{1:N}) = \sup_{[\boldsymbol{a},\boldsymbol{b}]}\left|\frac{1}{N}\sum_{n=1}^{N}\mathbb{1}\left(\mathbf{u}^n\in[\boldsymbol{a},\boldsymbol{b}]\right) - \prod_{i=1}^{d}(b_i-a_i)\right|$$

which is the discrepancy relative to the set $\mathcal{A}$ of $d-$dimensional intervals $[\boldsymbol{a},\boldsymbol{b}] := \prod_{i=1}^{d}[a_i,b_i]$, $0\le a_i<b_i<1$; and the star discrepancy:

$$D^\star(\mathbf{u}^{1:N}) = \sup_{[\mathbf{0},\boldsymbol{b}]}\left|\frac{1}{N}\sum_{n=1}^{N}\mathbb{1}\left(\mathbf{u}^n\in[\mathbf{0},\boldsymbol{b}]\right) - \prod_{i=1}^{d}b_i\right|,$$

where again $[\mathbf{0},\boldsymbol{b}] = \prod_{i=1}^{d}[0,b_i]$, $0<b_i<1$. When $d=1$, the star discrepancy is the Kolmogorov-Smirnov statistic for an uniformity test of the points $\mathbf{u}^n$.

These two discrepancies are related as follows (Niederreiter, 1992, Proposition 2.4):

$$D^\star(\mathbf{u}^{1:N}) \le D(\mathbf{u}^{1:N}) \le 2^d D^\star(\mathbf{u}^{1:N}).$$

The importance of the concept of discrepancy, and in particular of the star discrepancy, is highlighted by the Koksma–Hlawka inequality (see e.g. Kuipers and Niederreiter, 1974, Theorem 5.1):

$$\left|\frac{1}{N}\sum_{n=1}^{N}\varphi(\mathbf{u}^n) - \int_{[0,1)^d}\varphi(\mathbf{u})\,\mathrm{d}\mathbf{u}\right| \le V(\varphi)D^\star(\mathbf{u}^{1:N})$$

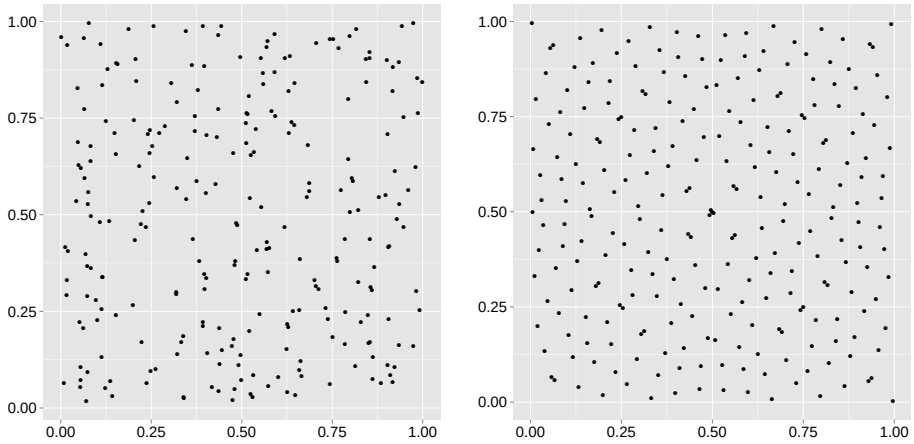

Figure 1.1: QMC versus Monte Carlo: $N = 256$ points sampled independently and uniformly in $[0,1)^2$ (left); QMC sequence (Sobol') in $[0,1)^2$ of the same length (right).

which conveniently separates the effect of the smoothness of φ (as measured by $V(\varphi)$, the total variation in the sense of Hardy and Krause, see Chapter 2 of Niederreiter, 1992 for a definition), and the effect of the discrepancy of the points $\mathbf{u}^{1:N}$. The quantity $V(\varphi)$ is generally too difficult to compute in practice, and the Koksma–Hlawka inequality is used mainly to determine the asymptotic error rate (as $N \to +\infty$), through the quantity $D^\star(\mathbf{u}^{1:N})$.

There are several methods to construct $\mathbf{u}^{1:N}$ so that $D^\star(\mathbf{u}^{1:N}) = \mathcal{O}(N^{-1+\epsilon})$ for any $\epsilon > 0$; which is of course better than the Monte Carlo rate $\mathcal{O}_P(N^{-1/2})$. The best known rates are $\mathcal{O}(N^{-1}(\log N)^{d-1})$ for QMC point sets $\mathbf{u}^{N,1:N}$ that are allowed to depend on N (i.e. $\mathbf{u}^{N,1:N}$ are not necessarily the N first elements of $\mathbf{u}^{N+1,1:N+1}$) and $\mathcal{O}(N^{-1}(\log N)^d)$ for QMC sequences (that is $\mathbf{u}^{1:N}$ are the N first elements of a sequence $(\mathbf{u}^n)$ which may be generated iteratively). For simplicity, we will not distinguish further QMC point sets and QMC sequences, and will use the same notation $\mathbf{u}^{1:N}$ in both cases (although our results will apply to both types of construction).

These asymptotic rates seem to indicate that the comparative performance of QMC over Monte Carlo should deteriorate with d: for $d = 10$, $N^{-1}(\log N)^d \leq N^{-1/2}$ only for $N \geq 1.3 \times 10^{39}$. But since these rates correspond to an upper bound for the error size, it is hard to determine beforehand if and when QMC "breaks" with the dimension. For instance, Glasserman (2004, p.327) exhibits a a numerical example where QMC remains competitive relative to Monte Carlo for $d \geq 150$ and $N \leq 10^5$.

Describing the different strategies to construct low-discrepancy point sets is beyond the scope of this paper; see again the aforementioned books on QMC. Figure 1.1 illustrates the greater regularity of a QMC point set over a set of random points.

1.1.3 Introduction to RQMC

RQMC (randomized QMC) amounts to randomize the points $\mathbf{u}^{1:N}$ in such a way that (a) they still have low discrepancy (with probability one); and (b) each $\mathbf{u}^n \sim \mathcal{U}([0,1)^d)$ marginally. The simplest construction of such RQMC point sets is the random shift method proposed by Cranley and Patterson (1976) in which we take $\mathbf{u}^n = \mathbf{v}^n + \mathbf{w} \pmod 1$, where $\mathbf{w} \sim \mathcal{U}([0,1)^d)$ and $\mathbf{v}^{1:N}$ is a low-discrepancy point set.

RQMC has two advantages over QMC. First, one then obtains an unbiased estimator of the integral of interest:

$$\mathbb{E}\left\{\frac{1}{N}\sum_{n=1}^{N}\varphi(\mathbf{u}^n)\right\} = \int_{[0,1)^d}\varphi(\mathbf{u})\,\mathrm{d}\mathbf{u},$$

which makes it possible to evaluate the approximation error through independent replications. We will see that, in our context, this unbiasedness property will also be very convenient for another reason: namely to provide an unbiased estimate of the likelihood of the considered state-space model.

Second, Owen (1997a,b, 1998) established that randomization may lead to better rates, in the following sense: under appropriate conditions, and for a certain type of randomization scheme known as nested scrambling, the mean square error of a RQMC estimator is $\mathcal{O}(N^{-3+\epsilon})$. The intuition behind this rather striking result is that randomization may lead to cancellation of certain error terms.

1.1.4 A note on array-RQMC

Consider the following problem: we have a Markov chain in $\mathcal{X}$, whose evolution may be formulated as

$$\mathbf{x}_t = \Gamma_t(\mathbf{x}_{t-1}, \mathbf{u}_t), \quad \mathbf{u}_t \sim \mathcal{U}\left([0,1)^d\right), \quad t \geq 1, \quad \mathbf{x}_0 \text{ is fixed},$$

and we wish to compute the expectation of $\sum_{t=1}^{T}\varphi_t(\mathbf{x}_t)$, for certain functions φ_t.

From the two previous sections, we see that a simple approach to this problem would be to generate a QMC (or RQMC) point set $\mathbf{u}^{1:N}$ in $[0,1)^{dT}$, $\mathbf{u}^n = (\mathbf{u}_1^n, \ldots, \mathbf{u}_T^n)$, to transform $\mathbf{u}_t^n$ into $\mathbf{x}_t^n = \Gamma_t(\mathbf{x}_{t-1}^n, \mathbf{u}_t^n)$, and finally to return the corresponding empirical average, $N^{-1}\sum_{t=1}^{T}\varphi_t(\mathbf{x}_t^n)$. The problem with this direct approach is that the dimension dT of $\mathbf{u}^{1:N}$ may be very large, and, as we have seen, equidistribution properties of QMC point sets (as measured by the star discrepancy) deteriorate with the dimension.

An elegant alternative to this approach is the array-RQMC algorithm of L'Ecuyer et al. (2006), see also Lécot and Ogawa (2002), Lécot and Tuffin (2004), and L'Ecuyer et al. (2009). The main idea of this method is to replace the QMC point set in $[0,1)^{dT}$ by T QMC points sets $\mathbf{u}_t^{1:N}$ in $[0,1)^d$. Then, $\mathbf{x}_t^n$ is obtained as $\mathbf{x}_t^n = \Gamma_t(\mathbf{x}_{t-1}^{a_{t-1}^n}, \mathbf{u}_t^n)$,

where the ancestor $\mathbf{x}_{t-1}^{a_{t-1}^n}$ of $\mathbf{x}_t^n$ is chosen so as to be the n-th "smallest" point among the $\mathbf{x}_{t-1}^n$'s. Note that array-RQMC therefore requires to specify a total order for the state space $\mathcal{X}$; for instance one may define a certain $\omega : \mathcal{X} \to \mathbb{R}$ so that $\omega(\mathbf{x}) \leq \omega(\mathbf{x}')$ means that $\mathbf{x}$ is "smaller" than $\mathbf{x}'$.

Array-RQMC is shown to have excellent empirical performance in the aforementioned papers. On the other hand, it is currently lacking in terms of supporting theory (see however L'Ecuyer et al., 2008, for $d = 1$); in particular, it is not clear how to choose the order ω, beside the obvious case where $\mathcal{X} \subset \mathbb{R}$. The SQMC algorithm we develop in this paper may be seen as an extension of array-RQMC to particle filtering. In particular, it re-uses the essential idea to generate one QMC point set at each step of the simulation process. As an added benefit, the convergence results we obtain for SQMC also apply to array-RQMC, provided the state space is ordered through the Hilbert curve, as explained later.

1.1.5 Background, plan and notations

QMC is already very popular in Finance for e.g. derivative pricing (Glasserman, 2004), and one may wonder why it has not received more attention in Statistics so far. The main reason seems to be the perceived difficulty to adapt QMC to non-independent simulation such as MCMC (Markov chain Monte Carlo); see however Chen et al. (2011) and references therein, in particular Tribble (2007), for exciting numerical and theoretical results in this direction which ought to change this perception.

Regarding SMC, we are aware of two previous attempts to develop QMC versions of these algorithms: Lemieux et al. (2001) and Fearnhead (2005); see also Guo and Wang (2006) who essentially proposed the same algorithm as Fearnhead (2005). The first paper casts SMC as a Monte Carlo algorithm in $d(T + 1)$ dimensions, where $d = \dim(\mathcal{X})$, and therefore requires to generate a low-discrepancy point set in $[0, 1)^{d(T+1)}$. But, as we have already explained, such an approach may not work well when $d(T + 1)$ is too large.

Our approach is closer to, and partly inspired by, the RPF (regularized particle filter) of Fearnhead (2005), who, in the same spirit as array-RQMC, casts SMC as a sequence of $T + 1$ successive importance sampling steps of dimension d. (The paper focus on the $d = 1$ case.) The main limitation of the RPF is that it has complexity $\mathcal{O}(N^2)$. This is because the importance sampling steps are defined with respect to a target which is a mixture of N components, hence the evaluation of a single importance weight costs $\mathcal{O}(N)$.

The SQMC algorithm we develop in this paper has complexity $\mathcal{O}(N \log(N))$ per time step. It is also based on a sequence of $T + 1$ importance sampling steps, but of dimension $d + 1$; the first component is used to determine which ancestor $\mathbf{x}_{t-1}^m$ should be assigned to particle $\mathbf{x}_t^n$. For $d > 1$, this requires us to "project" the set of ancestors $\mathbf{x}_{t-1}^{1:N} \in \mathcal{X}^N$ into $[0, 1)^N$, by means of a space-filling curve known

as the Hilbert curve. The choice of this particular space-filling curve is not only for computational convenience, but also because of its nice properties regarding conversion of discrepancy, as we will explain in the paper. (One referee pointed out to us that the use of Hilbert curve in the context of array-RQMC has been suggested by Wächter and Keller (2008), but not implemented.)

The paper is organised as follows. Section 1.2 derives the general SQMC algorithm, first for $d = 1$, then for any d through the use of the Hilbert curve. Section 1.3 presents several convergence results; proofs of these results are in the Appendix. Section 1.4 shows how several standard extensions of SMC, such as forward smoothing, backward smoothing, and PMCMC, may be adapted to SQMC. Section 1.5 compares numerically SQMC with SMC. Section 1.6 concludes.

Most random variables in this work will be vectors in $\mathbb{R}^d$, and will be denoted in bold face, $\mathbf{u}$ or $\mathbf{x}$. In particular, $\mathcal{X}$ will be an open set of $\mathbb{R}^d$. The Lebesgue measure in dimension d is denoted by λ_d. Let $\mathcal{P}(\mathcal{X})$ be the set of probability measures defined on $\mathcal{X}$ dominated by λ_d (restricted to $\mathcal{X}$), and $\pi(\varphi)$ be the expectation of function φ relative to $\pi \in \mathcal{P}(\mathcal{X})$. Let $a : b$ be the set of integers $\{a, \ldots, b\}$ for $a \leq b$. We also use this notation for collections of random variables, e.g. $\mathbf{x}_t^{1:N} = (\mathbf{x}_t^1, \ldots, \mathbf{x}_t^N)$, $\mathbf{x}_{0:t} = (\mathbf{x}_0, \ldots, \mathbf{x}_t)$ and so on.

1.2 SQMC

The objective of this section is to construct the SQMC algorithm. To this aim, we discuss how to rewrite SMC as a deterministic function of independent uniform variates $\mathbf{u}_t^{1:N}$, $t \in 0{:}T$, which then may be replaced by low-discrepancy point sets.

1.2.1 SMC formalisation

A closer inspection of our basic particle filter, Algorithm 1.1, reveals that this algorithm is entirely determined by (a) the sequence of proposal kernels $(m_t)_{t \geq 0}$ (which determine how particles are simulated) and (b) the sequence of weight functions $(G_t)_{t \geq 0}$ (which determine how particles are weighted). Our introduction to particle filtering focussed on the specific expression (1.1) for G_t, but useful SMC algorithms may be obtained by considering other weight functions; see e.g. the auxiliary particle filter of Pitt and Shephard (1999), as explained in Johansen and Doucet (2008), or the SMC algorithms for non-sequential problems mentioned in the introduction.

The exact expression and meaning of m_t and G_t will not play a particular role in the rest of the paper, so it is best to think of SMC from now on as a generic algorithm, again based on a certain sequence (m_t), $m_0(\mathrm{d}\mathbf{x}_0)$ being an initial distribution, and $m_t(\mathbf{x}_{t-1}, \mathrm{d}\mathbf{x}_t)$ being a Markov kernel for $t \geq 1$, and a certain sequence of functions, $G_0 : \mathcal{X} \to \mathbb{R}^+$, $G_t : \mathcal{X} \times \mathcal{X} \to \mathbb{R}^+$, which produces the following consistent (as

$N \to +\infty$) estimators:

$$\frac{1}{N}\sum_{n=1}^{N}\varphi(\mathbf{x}_t^n) \to \overline{\mathbb{Q}}_t(\varphi), \qquad \sum_{n=1}^{N} W_t^n \varphi(\mathbf{x}_t^n) \to \mathbb{Q}_t(\varphi),$$

where $\varphi : \mathcal{X} \to \mathbb{R}$, and $\overline{\mathbb{Q}}_t$ and $\mathbb{Q}_t$ are defined as follows:

$$Z_t = \mathbb{E}\left[G_0(\mathbf{x}_0)\prod_{s=1}^{t} G_s(\mathbf{x}_{s-1},\mathbf{x}_s)\right], \tag{1.2}$$

$$\overline{\mathbb{Q}}_t(\varphi) = \frac{1}{Z_{t-1}}\mathbb{E}\left[\varphi(\mathbf{x}_t)G_0(\mathbf{x}_0)\prod_{s=1}^{t-1} G_s(\mathbf{x}_{s-1},\mathbf{x}_s)\right], \tag{1.3}$$

$$\mathbb{Q}_t(\varphi) = \frac{1}{Z_t}\mathbb{E}\left[\varphi(\mathbf{x}_t)G_0(\mathbf{x}_0)\prod_{s=1}^{t} G_s(\mathbf{x}_{s-1},\mathbf{x}_s)\right], \tag{1.4}$$

with expectations taken with respect to the law of the non-homogeneous Markov chain $(\mathbf{x}_t)$, e.g.

$$Z_t = \int_{\mathcal{X}^{t+1}} \left\{G_0(\mathbf{x}_0)\prod_{s=1}^{t} G_s(\mathbf{x}_{s-1},\mathbf{x}_s)\right\} m_0(\mathrm{d}\mathbf{x}_0)\prod_{s=1}^{t} m_s(\mathbf{x}_{s-1},\mathrm{d}\mathbf{x}_s),$$

and with the conventions that $Z_{-1} = 1$ and empty products equal one; e.g. $\overline{\mathbb{Q}}_0(\varphi) = m_0(\varphi)$.

For instance, for the standard filtering problem covered in our introduction, where G_t is set to (1.1), $\mathbb{Q}_t(\varphi)$ is the filtering expectation of φ, i.e. $\mathbb{E}[\varphi(\mathbf{x}_t)|\mathbf{y}_{0:t}]$, and $\overline{\mathbb{Q}}_t(\varphi)$ is the predictive distribution of φ, i.e. $\mathbb{E}[\varphi(\mathbf{x}_t)|\mathbf{y}_{0:t-1}]$.

1.2.2 Towards SQMC: SMC as a sequence of importance sampling steps

QMC requires to write any simulation as an explicit function of uniform variates. We therefore make the following assumption for our generic SMC sampler: to generate $\mathbf{x}_0^n \sim m_0(\mathrm{d}\mathbf{x}_0)$, one computes $\mathbf{x}_0^n = \Gamma_0(\mathbf{u}_0^n)$, and to generate $\mathbf{x}_t^n|\mathbf{x}_{t-1}^n \sim m_t(\mathbf{x}_{t-1},\mathrm{d}\mathbf{x}_t)$, one computes $\mathbf{x}_t^n = \Gamma_t(\mathbf{x}_{t-1}^n,\mathbf{u}_t^n)$, where $\mathbf{u}_t^n \sim \mathcal{U}([0,1)^d)$, and the functions Γ_t are easy to evaluate.

Iteration 0 of Algorithm 1.1 amounts to an importance sampling step, from $m_0(\mathrm{d}\mathbf{x}_0)$ to $\mathbb{Q}_0(\mathrm{d}\mathbf{x}_0) = m_0(\mathrm{d}\mathbf{x}_0)G_0(\mathbf{x}_0)/Z_0$, which produces the following estimator

$$\sum_{n=1}^{N} W_0^n \varphi(\mathbf{x}_0^n) = \frac{\sum_{n=1}^{N} G_0(\mathbf{x}_0^n)\varphi(\mathbf{x}_0^n)}{\sum_{m=1}^{N} G_0(\mathbf{x}_0^m)}$$

of $\mathbb{Q}_0(\varphi)$. To introduce QMC at this stage, we take $\mathbf{x}_0^n = \Gamma_0(\mathbf{u}_0^n)$ where $\mathbf{u}_0^{1:N}$ is a low-discrepancy point set in $[0,1)^d$.

The key remark that underpins SQMC is that iteration $t \geq 1$ of Algorithm 1.1 also amounts to an importance sampling step, but this time from

$$\overline{\mathbb{Q}}_t^N(\mathrm{d}(\widetilde{\mathbf{x}}_{t-1}, \mathbf{x}_t)) = \sum_{n=1}^N W_{t-1}^n \delta_{\mathbf{x}_{t-1}^n}(\mathrm{d}\widetilde{\mathbf{x}}_{t-1}) m_t(\mathbf{x}_{t-1}^n, \mathrm{d}\mathbf{x}_t) \tag{1.5}$$

to

$$\mathbb{Q}_t^N(\mathrm{d}(\widetilde{\mathbf{x}}_{t-1}, \mathbf{x}_t)) = \frac{1}{\overline{\mathbb{Q}}_t^N(G_t)} \overline{\mathbb{Q}}_t^N(\mathrm{d}(\widetilde{\mathbf{x}}_{t-1}, \mathbf{x}_t)) G_t(\widetilde{\mathbf{x}}_{t-1}, \mathbf{x}_t)$$

where $\mathbb{Q}_t^N$ and $\overline{\mathbb{Q}}_t^N$ are two *random* probability measures defined over $\mathcal{X} \times \mathcal{X}$, a set of dimension $2d$. In particular, the generation of random variables $a_{t-1}^{1:N}$ and $\mathbf{x}_t^{1:N}$ in Steps (a) and (b) of Algorithm 1.1 is equivalent to sampling N times independently random variables $(\tilde{\mathbf{x}}_{t-1}^n, \mathbf{x}_t^n)$ from $\overline{\mathbb{Q}}_t^N(\mathrm{d}(\widetilde{\mathbf{x}}_{t-1}, \mathbf{x}_t))$: i.e. $\tilde{\mathbf{x}}_{t-1}^n = \mathbf{x}_{t-1}^{a_{t-1}^n}$ (not to be mistaken with $\mathbf{x}_{t-1}^n$), and $\mathbf{x}_t^n \sim m_t(\tilde{\mathbf{x}}_{t-1}^n, \mathrm{d}\mathbf{x}_t)$.

Based on these remarks, the general idea behind SQMC is to replace at iteration t the N IID random numbers sampled from $\overline{\mathbb{Q}}_t^N(\mathrm{d}(\widetilde{\mathbf{x}}_{t-1}, \mathbf{x}_t))$ by a low-discrepancy point set relative to the same distribution.

When $d = 1$, this idea may be implemented as follows: generate a low-discrepancy point set $\mathbf{u}_t^{1:N}$ in $[0,1)^2$, let $\mathbf{u}_t^n = (u_t^n, v_t^n)$, then set $\tilde{\mathbf{x}}_{t-1}^n = \hat{F}_N^{-1}(u_t^n)$, $\mathbf{x}_t^n = \Gamma_t(\tilde{\mathbf{x}}_{t-1}^n, v_t^n)$, where $\hat{F}_N^{-1}$ is the generalised inverse of the empirical CDF

$$\hat{F}_N(x) = \sum_{n=1}^N W_{t-1}^n \mathbb{1}\left\{\mathbf{x}_{t-1}^n \leq x\right\}, \quad x \in \mathcal{X} \subset \mathbb{R}.$$

It is easy to see that the most efficient way to compute $\tilde{\mathbf{x}}_{t-1}^n = \hat{F}_N^{-1}(u_t^n)$ for all $n \in 1{:}N$ is (a) to sort the $\mathbf{x}_{t-1}^n$'s, i.e. to find permutation σ such that $\mathbf{x}_{t-1}^{\sigma(1)} \leq \ldots \leq \mathbf{x}_{t-1}^{\sigma(N)}$, (b) to sort the $u_t^{1:N}$, call $\mathrm{sort}(u_t^{1:N})$ the corresponding result; (c) to obtain $a_{t-1}^{1:N}$ as the output of Algorithm 1.2, with inputs $\mathrm{sort}(u_t^{1:N})$ and $W_t^{\sigma(1:N)}$; and finally (d) set $\tilde{\mathbf{x}}_{t-1}^n = \mathbf{x}_{t-1}^{a_{t-1}^n}$.

Algorithm 1.3 gives a pseudo-code version of SQMC for any d, but note how Step (b) at times $t \geq 1$ simplifies to what we have just described for $d = 1$.

When $d > 1$, the inverse transform method cannot be used to sample from the marginal distribution of $\widetilde{\mathbf{x}}_{t-1}$ relative to $\overline{\mathbb{Q}}_t^N(\mathrm{d}(\widetilde{\mathbf{x}}_{t-1}, \mathbf{x}_t))$, at least unless the $\mathbf{x}_{t-1}^n$ are "projected" to the real line in some sense. This is the point of the Hilbert curve presented in the next section.

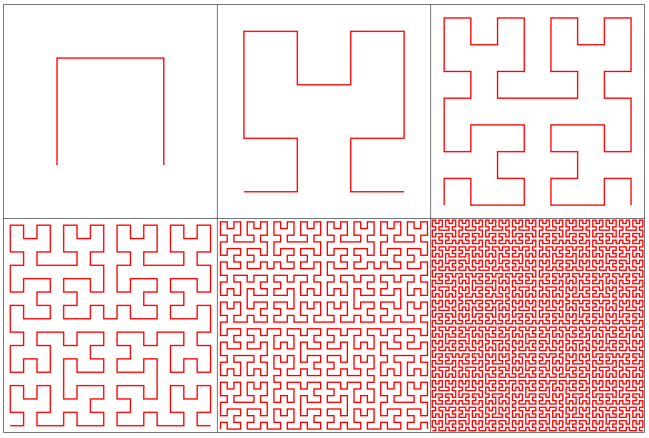

Figure 1.2: H_m curve for $d = 2$ and $m = 1$ to $m = 6$ (Source: Wikipedia)

1.2.3 The Hilbert space-filling curve

The Hilbert curve is a continuous fractal map $H : [0,1] \to [0,1]^d$, which "fills" entirely $[0,1]^d$. H is obtained as the limit of a sequence (H_m), $m \to +\infty$, the first terms of which are depicted in Figure 1.2.

The function H admits a pseudo-inverse $h : [0,1]^d \to [0,1]$, i.e. $H \circ h(\mathbf{x}) = \mathbf{x}$ for all $\mathbf{x} \in [0,1]^d$. H is not a bijection because certain points $\mathbf{x} \in [0,1]^d$ have more than one pre-image through H; however the set of such points is of Lebesgue measure 0.

Informally, H transforms $[0,1]$ into $[0,1]^d$, while preserving "locality": if x, $x' \in [0,1]$ are close, then $H(x)$ and $H(x')$ are close as well. We will establish that h also preserves discrepancy: a low-discrepancy point set in $[0,1)^d$ remains a low-discrepancy point set in $[0,1)$ when transformed through h. It is these properties that give to the Hilbert curve its appeal in the SQMC context (as opposed to other space filling curves, such as Z-ordering). We refer to Sagan (1994), Butz (1969) and Hamilton and Rau-Chaplin (2008) for how to compute h in practice for any $d \geq 2$. For $d = 1$, we simply set $H(x) = h(x) = x$ for $x \in [0,1]$.

The following technical properties of H and H_m will be useful later (but may be skipped on first reading). For $m \geq 0$, let $\mathcal{I}_m^d = \left\{I_m^d(k)\right\}_{k=0}^{2^{md}-1}$ be the collection of consecutive closed intervals in $[0,1]$ of equal size 2^{-md} and such that $\cup\mathcal{I}_m^d = [0,1]$. For $k \geq 0$, $S_m^d(k) = H_m(I_m^d(k))$ belongs to $\mathcal{S}_m^d$, the set of the 2^{md} closed hypercubes of volume 2^{-md} that covers $[0,1]^d$, $\cup\mathcal{S}_m^d = [0,1]^d$; $S_m^d(k)$ and $S_m^d(k+1)$ are adjacent, i.e. have at least one edge in common (*adjacency property*). If we split $I_m^d(k)$ into the 2^d successive closed intervals $I_{m+1}^d(k_i)$, $k_i = 2^d k + i$ and $i \in 0 : 2^d - 1$, then the $S_{m+1}^d(k_i)$'s are simply the splitting of $S_m^d(k)$ into 2^d closed hypercubes of volume $2^{-d(m+1)}$ (*nesting property*). Finally, the limit H of H_m has the *bi-measure property*: $\lambda_1(A) = \lambda_d(H(A))$ for any measurable set $A \subset [0,1]$, and satisfies the *Hölder condition* $\|H(x_1) - H(x_2)\|_\infty \leq C_H |x_1 - x_2|^{1/d}$ for any x_1, $x_2 \in [0,1]$.

1.2.4 SQMC for $d \geq 2$

Assume now $d \geq 2$, and consider the following change of variables at iteration $t \geq 1$:

$$h_{t-1}^n = h \circ \psi(\mathbf{x}_{t-1}^n) \in [0,1]$$

where $h : [0,1]^d \to [0,1]$ is the inverse of the Hilbert curve defined in the previous section, and $\psi : \mathcal{X} \to [0,1]^d$ is some user-chosen bijection between $\mathcal{X}$ and $\psi(\mathcal{X}) \subset [0,1]^d$. To preserve the low discrepancy property of $\mathbf{x}_{t-1}^{1:N}$ it is important to choose for ψ a mapping which is discrepancy preserving. This requires to select ψ such that $\psi(\mathbf{x}) = (\psi_1(x_1), ..., \psi_d(x_d))$ where the ψ_i's are continuous and strictly monotone. But choosing such a ψ is trivial in most applications; e.g. apply the logistic transformation component-wise when $\mathcal{X} = \mathbb{R}^d$ (see Section 1.5 for more details).

With this change of variables, we obtain particles $h_{t-1}^{1:N}$ that lie in $[0,1]$, and (1.5) becomes

$$\overline{\mathbb{Q}}_{t,h}^N \left(\mathrm{d}(\tilde{h}_{t-1}, \mathbf{x}_t) \right) = \sum_{n=1}^N W_{t-1}^n \delta_{h_{t-1}^n}(\mathrm{d}\tilde{h}_{t-1}) m_t(\mathbf{x}_{t-1}^n, \mathrm{d}\mathbf{x}_t).$$

Sampling a low-discrepancy sequence from $\overline{\mathbb{Q}}_{t,h}^N(\mathrm{d}\tilde{h}_{t-1}, \mathrm{d}\mathbf{x}_t)$ may then proceed exactly as for $d = 1$; that is: use the inverse transform method to sample N points $\tilde{h}_{t-1}^{1:N}$ from the marginal distribution $\overline{\mathbb{Q}}_{t,h}^N(\mathrm{d}\tilde{h}_{t-1})$, then sample $\mathbf{x}_t^{1:N}$ conditionally on $\tilde{\mathbf{x}}_{t-1}^{1:N}$, with $\tilde{\mathbf{x}}_{t-1}^n = \psi^{-1} \circ H(\tilde{h}_{t-1}^n)$. The exact details of the corresponding operations are the same as for $d = 1$. We therefore obtain the general SQMC algorithm as described in Algorithm 1.3.

To fully define SQMC, one must choose a particular method to generate point sets $\mathbf{u}_t^{1:N}$ at each iteration. If QMC point sets are generated, one obtains a deterministic algorithm, while if RQMC point sets are generated, one obtains a stochastic algorithm.

1.2.5 Complexity of SQMC

The complexity of both Steps (b) and (c) (for $t \geq 1$) of the SQMC algorithm is $\mathcal{O}(N \log N)$, because they include a sort operation. The complexity of Step (a) depends on the chosen method for generating the point sets $\mathbf{u}_t^{1:N}$. For instance, Hong and Hickernell (2003) propose a $\mathcal{O}(N \log N)$ method that applies to most constructions of (t,s)-sequences (such as the Faure, the Sobol', the Niederreiter or the Niederreiter-Xing sequences). The cost to randomize a QMC point set is only $\mathcal{O}(N)$ if one chooses the simple random shift approach, while nested scrambling methods for (t,s)-sequences, which are such that all the results below hold, may be implemented at cost $\mathcal{O}(N \log N)$ (Owen, 1995; Hong and Hickernell, 2003).

To summarise, the overall complexity of SQMC is $\mathcal{O}(N \log N)$, provided the method to generate the point sets $\mathbf{u}_t^{1:N}$ is chosen appropriately.

Algorithm 1.3 SQMC algorithm

At time $t = 0$,

(a) Generate a QMC or a RQMC point set $\mathbf{u}_0^{1:N}$ in $[0,1)^d$, and compute $\mathbf{x}_0^n = \Gamma_0(\mathbf{u}_0^n)$ for each $n \in 1:N$.

(b) Compute $w_0^n = G_0(\mathbf{x}_0^n)$ and $W_0^n = w_0^n / \sum_{m=1}^N w_0^m$ for each $n \in 1:N$.

Iteratively, from time $t = 1$ to time $t = T$,

(a) Generate a QMC or a RQMC point set $\mathbf{u}_t^{1:N}$ in $[0,1)^{d+1}$; let $\mathbf{u}_t^n = (u_t^n, \mathbf{v}_t^n) \in [0,1) \times [0,1)^d$.

(b) Hilbert sort: find permutation σ_{t-1} such that $h \circ \psi(\mathbf{x}_{t-1}^{\sigma_{t-1}(1)}) \leq \ldots \leq h \circ \psi(\mathbf{x}_{t-1}^{\sigma_{t-1}(N)})$ if $d \geq 2$, or $\mathbf{x}_{t-1}^{\sigma_{t-1}(1)} \leq \ldots \leq \mathbf{x}_{t-1}^{\sigma_{t-1}(N)}$ if $d = 1$.

(c) Find permutation τ such that $u_t^{\tau(1)} \leq ... \leq u_t^{\tau(N)}$, generate $a_{t-1}^{1:N}$ using Algorithm 1.2, with inputs $u_t^{\tau(1:N)}$ and $W_{t-1}^{\sigma_{t-1}(1:N)}$, and compute $\mathbf{x}_t^n = \Gamma_t(\mathbf{x}_{t-1}^{\sigma_{t-1}(a_{t-1}^n)}, \mathbf{v}_t^{\tau(n)})$ for each $n \in 1:N$.

(e) Compute $w_t^n = G_t(\mathbf{x}_{t-1}^{\sigma_{t-1}(a_{t-1}^n)}, \mathbf{x}_t^n)$, and $W_t^n = w_t^n / \sum_{m=1}^N w_t^m$ for each $n \in 1:N$.

1.3 Convergence study

We concentrate on two types of asymptotic results (as $N \to +\infty$): consistency, and stochastic bounds, that is bounds on the mean square error for the randomized SQMC algorithm (i.e. SQMC based on randomized QMC point sets). We leave deterministic bounds of the error (for when deterministic QMC point sets are used) to future work. We find stochastic bounds more interesting, because (a) results from (Owen, 1997a,b, 1998) suggest one might obtain better convergence rates than for deterministic bounds; and (b) the randomized version of SQMC has more applications, as discussed in Section 1.4.

These results are specialised to the case where the simulation of $\mathbf{x}_t^n$ at time t is based on the inverse transform method, as explained in Section 1.3.1. Certain of our results require $\mathcal{X}$ to be bounded, so for simplicity we take $\mathcal{X} = [0,1)^d$, and ψ is set to the identity function. (Recall that, to deal with certain QMC technicalities, we follow the standard practice of taking $\mathcal{X} = [0,1)^d$ rather than $\mathcal{X} = [0,1]^d$.) The fact that $\mathcal{X}$ is bounded may not be such a strong restriction, as our results allow for unbounded test functions φ; thus, one may accommodate for an unbounded state space (and expectations with respect to that space) through appropriate variable transforms.

We introduce the following extreme norm. For any signed measure μ over $\mathcal{X} = [0,1)^d$,

$$\|\mu\|_{\mathrm{E}} = \sup_{B \in \mathcal{B}_{[0,1)^d}} |\mu(B)|, \quad \mathcal{B}_{[0,1)^d} = \left\{ B : \; B = \prod_{i=1}^{d} [a_i, b_i] \subset [0,1)^d, \; a_i < b_i \right\}$$

which generalises the extreme discrepancy in the following sense:

$$\|\mathcal{S}(\mathbf{x}^{1:N}) - \lambda_d\|_{\mathrm{E}} = D(\mathbf{x}^{1:N})$$

for any point set $\mathbf{x}^{1:N}$ in $\mathcal{X}$, where $\mathcal{S}$ is the operator that associates to $\mathbf{x}^{1:N}$ its empirical distribution:

$$\mathbf{x}^{1:N} \in \mathcal{X}^N \mapsto \mathcal{S}(\mathbf{x}^{1:N}) = \frac{1}{N} \sum_{n=1}^{N} \delta_{\mathbf{x}^n}.$$

Our consistency results will be stated with this norm. Note that $\|\pi^N - \pi\|_{\mathrm{E}} \to 0$ implies $\left|\pi^N(\varphi) - \pi(\varphi)\right| \to 0$ for any continuous, bounded function φ, by portmanteau lemma (Van der Vaart, 2007, Lemma 2.2).

The next subsection explains how the inverse method may be used to generate $\mathbf{x}_t^n$ given $\mathbf{x}_{t-1}^n$. The two following subsections state preliminary results that should provide insights on the main ideas that underpin the proofs of our convergence results. Readers interested mostly in the main results may skip these subsections and go directly to Section 1.3.4 (consistency) and Section 1.3.5 (stochastic bounds).

This section will use the following standard notations: $\|\varphi\|_\infty$ for the supremum norm for functions φ, $L_2(\mathcal{X}, \mu)$ for the set of square integrable functions $\varphi : \mathcal{X} \to \mathbb{R}$ and $\mathcal{C}_b(\mathcal{X})$ for the set of continuous, bounded functions $\varphi : \mathcal{X} \to \mathbb{R}$.

1.3.1 Inverse transform method

We discuss here how to write the simulation of $\mathbf{x}_t^n$ as $\mathbf{x}_t^n = \Gamma_t(\mathbf{x}_{t-1}^n, \mathbf{u}_t^n)$, using the inverse transform method. Our convergence results are specialised to this particular Γ_t.

For a generic distribution $\pi \in \mathcal{P}(\mathcal{X})$, $\mathcal{X} \subset \mathbb{R}^d$, let F_π be the Rosenblatt transformation (Rosenblatt, 1952) of π defined through the following chain rule decomposition:

$$F_\pi(\mathbf{x}) = (u_1, \ldots, u_d)^T, \quad \mathbf{x} = (x_1, \ldots, x_d)^T \in \mathcal{X},$$

where, recursively, $u_1 = F_{\pi,1}(x_1)$, $F_{\pi,1}$ being the CDF of the marginal distribution of the first component (relative to π), and for $i \geq 2$, $u_i = F_{\pi,i}(x_i | x_{1:i-1})$, $F_{\pi,i}(\cdot | x_{1:i-1})$ being the CDF of component x_i, conditional on $(x_1, \ldots, x_{i-1})$, again relative to π. Similarly, we define the multivariate GICDF (generalised inverse CDF) F_π^{-1} through the following chain rule decomposition:

$$F_\pi^{-1}(\mathbf{u}) = (x_1, \ldots, x_d)^T, \quad \mathbf{u} = (u_1, \ldots, u_d)^T \in [0,1)^d,$$

where, recursively, $x_1 = F_{\pi,1}^{-1}(u_1)$, $F_{\pi,1}^{-1}$ being the GICDF of the marginal distribution of the first component (relative to π), and for $i \geq 2$, $x_i = F_{\pi,i}^{-1}(u_i|x_{1:i-1})$, $F_{\pi,i}^{-1}(\cdot|x_{1:i-1})$ being the GICDF of component x_i, conditional on $(x_1, \ldots, x_{i-1})$, again relative to π. Note that this function depends on the particular order of the components of π. For some probability kernel $K : \mathcal{X} \to \mathcal{P}(\mathcal{X})$, define similarly $F_K(\mathbf{x}, \cdot)$ and $F_K^{-1}(\mathbf{x}, \cdot)$ as, respectively, the Rosenblatt transformation and the multivariate GICDF of distribution $K(\mathbf{x}, \mathrm{d}\mathbf{x}')$ for a fixed $\mathbf{x}$.

It is well known that taking $\Gamma_0 = F_{m_0}^{-1}$, and $\Gamma_t = F_{m_t}^{-1}$ lead to valid simulations algorithms, i.e. if $\mathbf{x}_0^n = F_{m_0}^{-1}(\mathbf{u}_0^n)$, resp. $\mathbf{x}_t^n = F_{m_t}^{-1}(\mathbf{x}_{t-1}, \mathbf{u}_t^n)$, then $\mathbf{x}_0^n \sim m_0(\mathrm{d}\mathbf{x}_0)$, resp. $\mathbf{x}_t^n | \mathbf{x}_{t-1}^n \sim m_t(\mathbf{x}_{t-1}^n, \mathrm{d}\mathbf{x}_t)$.

1.3.2 Preliminary results: importance sampling

Since SQMC is based on importance sampling (e.g. Iteration 0 of Algorithm 1.3), we need to establish the validity of importance sampling based on low-discrepancy point sets; see Götz (2002); Aistleitner and Dick (2014) for other results on QMC-based importance sampling.

Theorem 1.1. *Let π and q be two probability measures on $[0,1)^d$ such that the Radon-Nikodym derivative $w(\mathbf{x}) = \pi(\mathrm{d}\mathbf{x})/q(\mathrm{d}\mathbf{x})$ is continuous and bounded. Let $(\mathbf{x}^{1:N})$ be a sequence of point sets in $[0,1)^d$ such that $\|\mathcal{S}(\mathbf{x}^{1:N}) - q\|_{\mathrm{E}} \to 0$ as $N \to +\infty$, and define*

$$\pi^N = \sum_{n=1}^N W^n \delta_{\mathbf{x}^n}, \quad W^n = \frac{w(\mathbf{x}^n)}{\sum_{m=1}^N w(\mathbf{x}^m)}.$$

Then, $\|\pi^N - \pi\|_{\mathrm{E}} \to 0$ as $N \to +\infty$.

See Section A.2 of the Appendix for a proof.

Recall that in our notations we drop the dependence of point sets on N, i.e. we write $(\mathbf{x}^{1:N})$ rather than $(\mathbf{x}^{N,1:N})$, although in full generality $\mathbf{x}^{1:N}$ may not necessarily be the N first points of a fixed sequence.

The next theorem gives the stochastic error rate when a RQMC point set is used.

Theorem 1.2. *Consider the set-up of Theorem 1.1. Let $(\mathbf{u}^{1:N})$ be a sequence of random point sets in $[0,1)^d$ such that $\mathbf{u}^n \sim \mathcal{U}([0,1)^d)$ marginally and, $\forall \varphi \in L_2([0,1)^d, \lambda_d)$,*

$$\mathrm{Var}\left(\frac{1}{N}\sum_{n=1}^N \varphi(\mathbf{u}^n)\right) = o\Big(r(N)\Big),$$

where $r(N) \to 0$ as $N \to +\infty$. Let $\mathbf{x}^{1:N} = F_q^{-1}(\mathbf{u}^{1:N})$ and assume that either one of the following two conditions is verified:

1. *F_q^{-1} is continuous and, for any $\epsilon > 0$, there exists a $N_\epsilon \in \mathbb{N}$ such that, almost surely, $D^\star(\mathbf{u}^{1:N}) \leq \epsilon$, $\forall N \geq N_\epsilon$;*

2. for any $\epsilon > 0$ there exists a $N_\epsilon \in \mathbb{N}$ such that, almost surely,

$$\|\mathcal{S}(\mathbf{x}^{1:N}) - q\|_{\mathrm{E}} \leq \epsilon, \quad \forall N \geq N_\epsilon.$$

Then, for all $\varphi \in L_2(\mathcal{X}, \pi)$,

$$\mathbb{E}\left|\pi^N(\varphi) - \pi(\varphi)\right| = o\Big(r(N)^{1/2}\Big), \quad \mathrm{Var}\left(\pi^N(\varphi)\right) = o\Big(r(N)\Big).$$

See Section A.2 of the Appendix for a proof.

To fix ideas, note that several RQMC strategies reach the Monte Carlo error rate and therefore fulfil the assumptions above with $r(N) = N^{-1+\epsilon}$ for any $\epsilon > 0$ (see e.g. Owen, 1997a, 1998). In addition, nested scrambling methods for (t, s)-sequences in base b (Owen, 1995; Matoŭsek, 1998; Hong and Hickernell, 2003) are such that $r(N) = N^{-1}$. This result is established for $N = \lambda b^m$ in Owen (1997a, 1998) and extended for an arbitrary N in Gerber (2014).

1.3.3 Preliminary results: Hilbert curve and discrepancy

We motivated the use of the Hilbert curve as a way to transform back and forth between $[0,1]^d$ and $[0,1]$ while preserving low discrepancy in some sense. This section formalises this idea.

For a probability measure π on $[0,1)^d$, we write π_h the image by h of π. For a kernel $K : [0,1)^d \to \mathcal{P}(\mathcal{X})$, we write $\pi_h \otimes K_h\left(\mathrm{d}(h_1, \mathbf{x}_2)\right)$ the image of $\pi \otimes K$ by the mapping $(\mathbf{x}_1, \mathbf{x}_2) \in [0,1)^d \times \mathcal{X} \mapsto (h(\mathbf{x}_1), \mathbf{x}_2)$, where $\pi \otimes K$ denotes the joint probability measure $\pi(\mathrm{d}\mathbf{x}_1)K(\mathbf{x}_1, \mathrm{d}\mathbf{x}_2)$.

The following theorem is a technical result on the conversion of discrepancy through h.

Theorem 1.3. *Let (π^N) be a sequence of probability measure on $[0,1)^d$ such that, $\|\pi^N - \pi\|_{\mathrm{E}} \to 0$, where $\pi(\mathrm{d}\mathbf{x}) = \pi(\mathbf{x})\lambda_d(\mathrm{d}\mathbf{x})$ admits a bounded probability density $\pi(\mathbf{x})$. Then*

$$\|\pi_h^N - \pi_h\|_{\mathrm{E}} \to 0, \quad \text{as } N \to +\infty.$$

See Section B.1 of the Appendix for a proof.

The following theorem is an extension of Hlawka and Mück (1972, "Satz 2"), which establishes the validity, in the context of QMC, of the multivariate GICDF approach described in Section 1.3.1. More precisely, for a probability measure π on $[0,1)^d$, Hlawka and Mück (1972, "Satz 2") show that $\|\mathcal{S}\left(F_\pi^{-1}(\mathbf{u}^{1:N})\right) - \pi\|_{\mathrm{E}} \leq cD^\star(\mathbf{u}^{1:N})^{1/d}$ (under some conditions on F_π, see below).

Theorem 1.4. *Let $K : [0,1)^{d_1} \to \mathcal{P}\left([0,1)^{d_2}\right)$ be a Markov kernel and assume that:*

1. *For a fixed $\mathbf{x}_1 \in [0,1)^{d_1}$, the i-th coordinate of $F_K\left(\mathbf{x}_1, \mathbf{x}_2\right)$ is strictly increasing in $x_{2i} \in [0,1)$, $i \in 1 : d_2$, and, viewed as a function of $\mathbf{x}_1$ and $\mathbf{x}_2$, $F_K\left(\mathbf{x}_1, \mathbf{x}_2\right)$ is Lipschitz;*

2. $\pi^N(\mathrm{d}\mathbf{x}) = \sum_{n=1}^N W_N^n \delta_{\mathbf{x}_1^n}(\mathrm{d}\mathbf{x})$, $\mathbf{x}_1^n \neq \mathbf{x}_1^m$ $\forall n \neq m \in 1:N$, *and* $\max_{n\in 1:N} W_N^n \to 0$.

3. *The sequence* (π^N) *is such that* $\|\pi^N - \pi\|_{\mathrm{E}} \to 0$ *as* $N \to +\infty$, *where* $\pi(\mathrm{d}\mathbf{x}) = \pi(\mathbf{x})\lambda_{d_1}(\mathrm{d}\mathbf{x})$ *admits a strictly positive bounded density* π.

Let $(\mathbf{u}^{1:N})$, $\mathbf{u}^n = (u^n, \mathbf{v}^n) \in [0,1)^{1+d_2}$, *be a sequence of point sets in* $[0,1)^{1+d_2}$ *such that* $D^\star(\mathbf{u}^{1:N}) \to 0$ *as* $N \to +\infty$, *and define* $P_h^N = \left(h^{1:N}, \mathbf{x}_2^{1:N}\right)$ *where*

$$h^n = F^{-1}_{\pi_h^N}(u^n), \quad \tilde{\mathbf{x}}_1^n = H(h^n), \quad \mathbf{x}_2^n = F_K^{-1}\left(\tilde{\mathbf{x}}_1^n, \mathbf{v}^n\right).$$

Then

$$\|\mathcal{S}(P_h^N) - \pi_h^N \otimes K_h\|_{\mathrm{E}} \to 0, \quad \text{as } N \to +\infty.$$

See Section B.2 of the Appendix for a proof.

Assumption 1 regarding the regularity of the vector-valued function F_K is the main assumption of the above theorem and comes from Hlawka and Mück (1972, "Satz 2"). It is verified as soon as kernel K admits a density that is continuously differentiable on $[0,1)^d$ (Hlawka and Mück, 1972, p.232). Assumption 2 is a technical condition, which will always hold under the assumptions of our main results.

1.3.4 Consistency

We are now able to establish the consistency of SQMC; see Appendix C for a proof of the following theorem. For convenience, let $F_{m_t}(\mathbf{x}_{t-1}, \mathbf{x}_t) = F_{m_0}(\mathbf{x}_0)$ when $t = 0$.

Theorem 1.5. *Consider the set-up of Algorithm 1.3 where, for all* $t \in 0:T$, $(\mathbf{u}_t^{1:N})$ *is a (non random) sequence of point sets in* $[0,1)^{d_t}$, *with* $d_0 = d$ *and* $d_t = d+1$ *for* $t > 0$, *such that* $D^\star(\mathbf{u}_t^{1:N}) \to 0$ *as* $N \to +\infty$. *Assume the following holds for all* $t \in 0{:}T$:

1. *The components of* $\mathbf{x}_t^{1:N}$ *are pairwise distinct,* $\mathbf{x}_t^n \neq \mathbf{x}_t^m$ *for* $n \neq m$.

2. G_t *is continuous and bounded;*

3. $F_{m_t}(\mathbf{x}_{t-1}, \mathbf{x}_t)$ *verifies Assumption 1 of Theorem 1.4 ;*

4. $\mathbb{Q}_t(\mathrm{d}\mathbf{x}_t) = p_t(\mathbf{x}_t)\lambda_d(\mathrm{d}\mathbf{x}_t)$ *where* $p_t(\mathbf{x}_t)$ *is a strictly positive bounded density.*

Let $\widehat{\mathbb{Q}}_t^N(\mathrm{d}\mathbf{x}_t) = \sum_{n=1}^N W_t^n \delta_{\mathbf{x}_t^n}(\mathrm{d}\mathbf{x}_t)$. *Then, under Assumptions 1-4, as* $N \to +\infty$,

$$\|\widehat{\mathbb{Q}}_t^N - \mathbb{Q}_t\|_{\mathrm{E}} \to 0, \quad \forall t \in 0{:}T.$$

Assumption 1 is stronger than necessary because for the result to hold it is enough that the number of identical particles does not grow too quickly as $N \to +\infty$. Note that this is a very weak restriction since Assumption 1 holds almost surely when RQMC point sets are used, since then the particles are generated from a continuous GICDF. The assumption that the weight functions (G_t) are bounded is standard in SMC literature (see e.g. Del Moral, 2004).

1.3.5 Stochastic bounds

Our second main result concerns stochastic bounds for the randomized version of SQMC, i.e. SQMC based on randomized point sets $(\mathbf{u}_t^n)$. See Section D of the Appendix for a proof of the next result.

Theorem 1.6. *Consider the set-up of Algorithm 1.3 where* $(\mathbf{u}_t^{1:N})$, $t \in 0:T$, *are independent sequences of random point sets in* $[0,1)^{d_t}$, *with* $d_0 = d$ *and* $d_t = d+1$ *for* $t > 0$, *such that, for all* $t \in 0:T$, $\mathbf{u}_t^n \sim \mathcal{U}([0,1)^{d_t})$ *marginally and*

1. *For any* $\epsilon > 0$, *there exists a* $N_{\epsilon,t} > 0$ *such that, almost surely,* $D^\star(\mathbf{u}_t^{1:N}) \leq \epsilon$, $\forall N \geq N_{\epsilon,t}$.

2. *For any function* $\varphi \in L_2\left([0,1)^{d_t}, \lambda_{d_t}\right)$, $\mathrm{Var}\left(\frac{1}{N}\sum_{n=1}^N \varphi(\mathbf{u}_t^n)\right) \leq C^* \sigma_\varphi^2 r(N)$ *where* $\sigma_\varphi^2 = \int \left\{\varphi(\mathbf{u}) - \int \varphi(\mathbf{v})\mathrm{d}\mathbf{v}\right\}^2 \mathrm{d}\mathbf{u}$, *and where both* C^* *and* $r(N)$ *do not depend on* φ.

In addition, assume that the Assumptions of Theorem 1.5 are verified and that $F_{m_0}^{-1}$ *is continuous. Let* $\varphi \in L_2([0,1)^d, \mathbb{Q}_t)$ *for all* $t \in 0{:}T$. *Then,* $\forall t \in 0{:}T$,

$$\mathbb{E}\left|\widehat{\mathbb{Q}}_t^N(\varphi) - \mathbb{Q}_t(\varphi)\right| = \mathcal{O}\Big(r(N)^{1/2}\Big), \quad \mathrm{Var}\Big(\widehat{\mathbb{Q}}_t^N(\varphi)\Big) = \mathcal{O}\Big(r(N)\Big).$$

Note that the implicit constants in the line above may depend on φ. Assumptions 1 and 2 are verified for $r(N) = N^{-1}$ if $\mathbf{u}_t^{1:N}$ is the first N points of a nested scrambled (t,s)-sequences in base $b \geq 2$. This result is established for $N = \lambda b^m$ in Owen (1997a, 1998) and can be extended to any pattern of N using Hickernell and Yue (2001, Lemma 1). Consequently, for this construction of RQMC point sets, Theorem 1.6 shows that the approximation error of SQMC goes to zero at least as fast as for SMC. However, contrary to the $\mathcal{O}(N^{-1})$ convergence rate of SMC, this rate for SQMC based on nested scrambled (t,s)-sequences is not exact but results from a worst case analysis. We can therefore expect to reach faster convergence on a smaller class of functions. The following result shows that it is indeed the case on the class on continuous and bounded functions; see Section D.4 of the Appendix for a proof.

Theorem 1.7. *Consider the set-up of Algorithm 1.3 where* $(\mathbf{u}_t^{1:N})$, $t \in 0{:}T$, *are* (t, d_t)*-sequences in base* $b \geq 2$, *with* $d_0 = d$ *and* $d_t = d+1$ *for* $t > 0$, *independently scrambled such that results in Owen (1997a, 1998) hold. Let* $N = \lambda b^m$, $1 \leq \lambda < b$, *and assume the following holds:*

1. *Assumptions of Theorem* (1.6) *are verified;*

2. *For* $t \in 1{:}T$, $F_{m_t}^{-1}(\mathbf{x}_{t-1}, \mathbf{x}_t)$ *is a continuous function of* $\mathbf{x}_{t-1}$.

Let $\varphi \in \mathcal{C}_b(\mathcal{X})$. *Then,* $\forall t \in 0{:}T$,

$$\mathbb{E}|\widehat{\mathbb{Q}}_t^N(\varphi) - \mathbb{Q}_t(\varphi)| = o(N^{-1/2}), \quad \mathrm{Var}(\widehat{\mathbb{Q}}_t^N(\varphi)) = o(N^{-1}).$$

Thus, for SQMC based on the first $N = \lambda b^m$ points of nested scrambled (t, s)-sequences in base b, one obtains that the stochastic error of (the random version of) SQMC converges faster than for SMC. Note that we can relax the constraint on N in Theorem 1.7 using Gerber (2014, Corollary 2).

1.4 Extensions

1.4.1 Unbiased estimation of evidence, PMCMC

Like SMC, the randomized version of SQMC (that is SQMC based on RQMC point sets) provides an unbiased estimator of the normalising constant Z_t of the Feynman-Kac model, see (1.2).

Lemma 1.1. *Provided that $\mathbf{u}_t^{1:N}$ is a RQMC point set in $[0,1)^{d_t}$ for $t \in 0:T$ (i.e. $\mathbf{u}_t^n \sim \mathcal{U}([0,1)^{d_t})$ marginally), with $d_0 = d$ and $d_t = d+1$ for $t > 0$, the following quantity*

$$Z_t^N = \left\{ \frac{1}{N} \sum_{n=1}^N G_0(\mathbf{x}_0^n) \right\} \prod_{s=1}^t \left\{ \frac{1}{N} \sum_{n=1}^N G_s(\mathbf{x}_{s-1}^{a_{s-1}^n}, \mathbf{x}_s^n) \right\}$$

is an unbiased estimator of Z_t, $\mathbb{E}[Z_t^N] = Z_t$.

We omit the proof, as it follows the same steps as for SMC (Del Moral, 1996).

In a state-space model parametrised by $\theta \in \Theta$, $Z_t = Z_t(\theta)$ is the marginal likelihood of the data up to time t. One may want to implement a Metropolis-Hastings sampler with respect to posterior density $\pi_T(\theta) \propto p(\theta) Z_T(\theta)$ for the full dataset and for a prior distribution $p(\theta)$, but $Z_T(\theta)$ is typically intractable.

Andrieu et al. (2010) established that, by substituting $Z_T(\theta)$ with an unbiased estimate of $Z_T(\theta)$ in a Metropolis sampler, one obtains an exact MCMC (Markov chain Monte Carlo) algorithm, in the sense that the corresponding MCMC kernel leaves invariant $\pi_T(\theta)$. The so obtained algorithm is called PMMH (Particle marginal Metropolis-Hastings). Andrieu et al. (2010) use SMC to obtain an unbiased estimate of $Z_T(\theta)$, that is, at each iteration a SMC sampler is run to obtain that estimate. We will call PMMH-SQMC the same algorithm, but with SQMC replacing SMC for the evaluation of an unbiased estimate of the likelihood.

The acceptance rate of PMMH depends directly on the variability of the estimates of $Z_T(\theta)$. Since the point of (randomized) SQMC is to provide estimates with a lower variance than SMC (for a given N), one may expect that PMMH-SQMC may require a smaller number of particles than standard PMMH for satisfactory acceptance rates; see Section 1.5 for a numerical illustration of this.

1.4.2 Smoothing

Smoothing amounts to compute expectations $\mathbb{Q}_t(\varphi)$ of functions φ of the complete trajectory $\mathbf{x}_{0:t}$; e.g. $\mathbb{Q}_t(\varphi)$ is the expectation of $\varphi(\mathbf{x}_{0:t})$ conditional on data $\mathbf{y}_{0:t}$ for a state-space model with Markov process $(\mathbf{x}_t)$ and observed process $(\mathbf{y}_t)$. See Briers et al. (2010) for a general overview on SMC smoothing algorithms. This section discusses how to adapt certain of these algorithms to SQMC.

Forward smoothing

Forward smoothing amounts to carry forward the complete trajectories of the particles, rather than simply keeping the last component $\mathbf{x}_t^n$ (as in Algorithm 1.1). A simple way to formalise forward smoothing is to introduce a path Feynman-Kac model, corresponding to the inhomogeneous Markov process $\mathbf{z}_t = \mathbf{x}_{0:t}$, and weight function (abusing notations) $G_t(\mathbf{z}_t) = G_t(\mathbf{x}_t)$. Then forward smoothing amounts to Algorithm 1.1 applied to this path Feynman-Kac model (substituting $\mathbf{x}_t$ with $\mathbf{z}_t = \mathbf{x}_{0:t}$).

One may use the same remark to define a SQMC version of forward smoothing: i.e. simply apply SQMC to the same path Feynman-Kac model. The only required modification is that the Hilbert sort of Step (b) at times $t \geq 1$ must now operate on some transformation of the vectors $\mathbf{z}_t^n$, of dimension $(t+1)d$, rather than vectors $\mathbf{x}_t^n$ of dimension d as in the original version.

Forward smoothing is sometimes used to approximate the smoothing expectation of additive functions, $\varphi(\mathbf{x}_{0:t}) = \sum_{s=0}^{t} \tilde{\varphi}(\mathbf{x}_s)$, such as the score function of certain models (e.g. Poyiadjis et al., 2011). In that case, one may instead apply SQMC to the Feynman-Kac model corresponding to the inhomogeneous Markov process $\mathbf{z}_t = (\sum_{s=0}^{t-1} \tilde{\varphi}(\mathbf{x}_s), \mathbf{x}_t)$. This means that in practice, one may implement the Hilbert sort on a space of much lower dimension (i.e. the dimension of this new $\mathbf{z}_t$), which is computationally more convenient.

Backward smoothing

Backward smoothing consists of two steps: (a) a forward pass, where SMC is run from time 0 to time T; and (b) a backward pass, where one constructs a trajectory $\tilde{\mathbf{x}}_{0:T}$ recursively backwards in time, by selecting randomly each component $\tilde{\mathbf{x}}_t$ out of the N particle values $\mathbf{x}_t^n$ generated during the forward pass. An advantage of backward smoothing is that it is less prone to degenerate than forward smoothing. A drawback of backward smoothing is that generating a single trajectory costs $\mathcal{O}(N)$, hence obtaining N of them costs $\mathcal{O}(N^2)$.

Backward smoothing for SQMC may be implemented in a similar way to SMC: see Algorithm 1.4 for the backward pass that generates N_B trajectories $\tilde{\mathbf{x}}_{0:T}^{1:N_B}$ from the output of the SQMC algorithm. Note that backward smoothing requires that the Markov kernel $m_t(\mathbf{x}_{t-1}, \mathrm{d}\mathbf{x}_t)$ admits a closed-form density $m_t(\mathbf{x}_t|\mathbf{x}_{t-1})$ with respect

Algorithm 1.4 Backward step of SQMC backward smoothing

Input: $\mathbf{x}_{0:T}^{\sigma_t(1:N)}$, $W_{0:T}^{\sigma_t(1:N)}$ (output of SQMC obtained after the Hilbert sort step, i.e for all $t \in 0{:}T$, $h \circ \psi(\mathbf{x}_t^{\sigma_t(n)}) \leq h \circ \psi(\mathbf{x}_t^{\sigma_t(m)})$, $n \leq m$) and $\tilde{\mathbf{u}}^{1:N_B}$ a point set in $[0,1)^{T+1}$; let $\tilde{\mathbf{u}}^n = (\tilde{u}_0^n, \ldots, \tilde{u}_T^n)$.

Output: $\tilde{\mathbf{x}}_{0:T}^{1:N_B}$ (N_B trajectories in $\mathcal{X}^{T+1}$)

Find permutation τ such that $\tilde{u}_0^{\tau(1)} \leq ... \leq \tilde{u}_0^{\tau(N_B)}$, generate $\tilde{a}_T^{1:N_B}$ using Algorithm 1.2, with inputs $\tilde{u}_0^{\tau(1:N_B)}$ and $W_T^{\sigma_T(1:N)}$, and set $\tilde{\mathbf{x}}_T^n = \mathbf{x}_T^{\tilde{a}_T^n}$ for all $n \in 1:N_B$.

for $t = T-1 \to 0$ **do**

For $n \in 1:N_B$, set $\tilde{\mathbf{x}}_t^n = \mathbf{x}_t^{\tilde{a}_t^n}$ where $\tilde{a}_t^n = F_{\pi_t^n}^{-1}(\tilde{u}_{T-t}^{\tau(n)})$, $\pi_t^n = \sum_{m=1}^N \widetilde{W}_t^m(\tilde{\mathbf{x}}_{t+1}^n)\delta_m$ and, for $m \in 1:N$,

$$\widetilde{W}_t^m(\mathbf{x}_{t+1}) = W_t^{\sigma_t(m)} m_t(\mathbf{x}_{t+1}|\mathbf{x}_t^{\sigma_t(m)}) / \left\{ \sum_{n=1}^N W_t^n m_t(\mathbf{x}_{t+1}|\mathbf{x}_t^n) \right\}.$$

end for

to an appropriate dominating measure. Then one may compute empirical averages over the so obtained N_B trajectories to obtain smoothing estimates in the usual way.

1.5 Numerical study

The objective of this section is to compare the performance of SMC and SQMC. Our comparisons are either for the same number of particles N, or for the same amount of CPU time to take into account the fact that SQMC has greater complexity than SMC. These comparisons will often summarised through gain factors, which we define as ratios of mean square errors (for a certain quantity) between SMC and SQMC.

In SQMC, we generate $\mathbf{u}_t^{1:N}$ as a Owen (1995) nested scrambled Sobol' sequence using the C++ library of T. Kollig and A. Keller (`http://www.uni-kl.de/AG-Heinrich/SamplePack.html`). Note that both the generation and the randomization of (t,s)-sequences in base 2 (such as the Sobol' sequence) are very fast since logical operations can be used. In order to sort the particles according to their Hilbert index we use the C++ library of Chris Hamilton (`http://web.cs.dal.ca/~chamilto/hilbert/index.html`) to evaluate $H_m^{-1}(\psi(\mathbf{x}))$, $m \in \mathbb{N}$. Again, Hilbert computations are very fast as they are based on logical operations (see Hamilton and Rau-Chaplin, 2008, for more details). In addition, thanks to the nesting property of the Hilbert curve (see Section 1.2.3) we only need to take m large enough such that different particles are mapped into different points of $[0,1)$. Function Γ_t is set to the inverse transform described in Section 1.3.1, and function ψ to a component-wise

(rescaled) logistic transform; that is, $\psi(\mathbf{x}) = (\psi_1(x_1), ..., \psi_d(x_d))$ with

$$\psi_i(x_i) = \left[1 + \exp\left(-\frac{x_i - \underline{x}_i}{\bar{x}_i - \underline{x}_i}\right)\right]^{-1}, \quad i \in 1:d$$

and where the constants $\bar{x}_i$ and $\underline{x}_i$ are used to solve numerical problems due to high values of $|x_i|$. For instance, when $(\mathbf{x}_t)$ is a stationary process we chose $\bar{x}_i = \mu_i + 2\sigma_i$ and $\underline{x}_i = \mu_i - 2\sigma_i$ where μ_i and σ^2 are respectively the mean and the standard deviation of the stationary distribution of $(\mathbf{x}_t)$.

SMC is implemented using systematic resampling (Carpenter et al., 1999) and all the random variables are generated using standard methods (i.e. not using the multivariate GICDF). The C/C++ code implementing both SMC and SQMC is available on-line at `https://bitbucket.org/mgerber/sqmc`.

Even if Theorems 1.6 and 1.7 are valid for any pattern of N, choosing for N powers of 2 (with 2 the base of the Sobol' sequence) is both natural and optimal for QMC methods based on (scrambled) (t, s)-sequences (see e.g. Owen, 1997b; Hickernell and Yue, 2001; and Chapter 5 of Dick and Pillichshammer, 2010). Comparing the performance of SQMC for different patterns of N is beyond the scope of this paper (see Gerber, 2014, for a discussion of this point) and therefore we follow in this numerical study the standard approach in the QMC literature by considering values of N that are powers of 2. We nevertheless do one exception to this rule for the PMMH estimation on real data (Section 1.5.3) because doubling the number of particles to reduce the variance of the likelihood estimate used in the Metropolis-Hastings ratio may be very inefficient from a computational point of view. As we will see, allowing N to differ from powers of the Sobol' base does not seem to alter the performance of SQMC.

One may expect the two following situations to be challenging for SQMC: (a) small N (because our results are asymptotic); and (b) large d (because of the usual deterioration of QMC with respect of the dimension, and also because of the Hilbert sort step). Thus we consider examples of varying dimensions (from 1 to 10), and we will also make N vary within a large range (between 2^4 and 2^{17}).

1.5.1 Example 1: A non linear and non stationary univariate model

We consider the following popular toy example (Gordon et al., 1993; Kitagawa, 1996):

$$\begin{cases} y_t = \frac{x_t^2}{a} + \epsilon_t, & \epsilon_t \sim \mathcal{N}_1(0,1), \quad t \geq 0 \\ x_t = b_1 x_{t-1} + b_2 \frac{x_{t-1}}{1+x_{t-1}^2} + b_3 \cos(b_4 t) + \sigma \nu_t, & \nu_t \sim \mathcal{N}_1(0,1), \quad t > 0 \end{cases} \tag{1.6}$$

and $x_0 \sim \mathcal{N}_1(0, 2)$, where $\mathcal{N}_d(\boldsymbol{\mu}, \Sigma)$ denotes the d-dimensional Gaussian distribution with mean $\boldsymbol{\mu}$ and covariance matrix Σ. We generate observations from 100 time

steps of the model, with the parameters set as in Gordon et al. (1993): $a = 20$, $\boldsymbol{b} = (0.5, 25, 8, 1.2)$, $\sigma^2 = 10$, $x_0 = 0.1$. Note that inference in this model is non trivial because the observation y_t does not allow to identify the sign of x_t, and because the weight function $G_t(x_t)$ is bimodal if $y_t > 0$ (with modes at $\pm(20y_t)^{1/2}$). In addition, we expect this model to be challenging for SQMC due to the high non linearity of the Markov transition $m_t(\mathbf{x}_{t-1}, \mathrm{d}\mathbf{x}_t)$.

All the results presented below are based on 500 independent runs of SMC and SQMC. Figure 1.4 presents results concerning the estimation of the log-likelihood functions evaluated at the true value of the parameters. The two top graphs show that, compared to SMC, SQMC yields faster convergence of both the mean and the variance of the estimates.

These better consistency properties of SQMC are also illustrated on the bottom left graph of Figure 1.4 where we have reported for each N the range in which lies the 500 estimates of the log-likelihood. From this plot we see that quickly the SQMC estimates stay in a very tiny interval while, on the contrary, the SMC estimates are much more dispersed, even for large values of N.

The bottom right panel of Figure 1.4 shows the MSE of SQMC and SMC as a function of CPU time. One sees that the gain of SQMC over SMC does not only increase with N, as predicted by the theory, but also with the CPU time which is of more practical interest. On the other hand, in this particular case (log-likelihood evaluation for this univariate model), when N is small the reduction in MSE brought by SQMC does not compensate its greater running time. Nevertheless, we observe that SQMC outperforms SMC very quickly, that is, as soon as the CPU time is larger or equal to $10^{-1.5} \approx 0.03$ seconds.

In the left graph of Figure 1.3 we have reported the gain factor for the estimation of $\mathbb{E}[x_t|y_{0:t}]$ as a function of t and for different values of N. From this plot we observe both significant and increasing gain of SQMC over SMC.

The right panel of Figure 1.3 compares SQMC and SMC backward smoothing for the estimation of $\mathbb{E}[x_t|y_{0:T}]$ as a function of t and for $N \in \{2^7, 2^9\}$. As for the filtering problem, SQMC significantly outperforms SMC with gain factors that increase with the number of particles.

1.5.2 Example 2: Multivariate stochastic volatility model

We consider the following multivariate stochastic volatility model (SV) proposed by Chan et al. (2006):

$$\begin{cases} \mathbf{y}_t = S_t^{1/2} \boldsymbol{\epsilon}_t, & t \geq 0 \\ \mathbf{x}_t = \boldsymbol{\mu} + \Phi(\mathbf{x}_{t-1} - \boldsymbol{\mu}) + \Psi^{\frac{1}{2}} \boldsymbol{\nu}_t, & t > 0 \end{cases} \tag{1.7}$$

where $S_t = \mathrm{diag}(\exp(x_{t1}), ..., \exp(x_{td}))$, Φ and Ψ are diagonal matrices and $(\boldsymbol{\epsilon}_t, \boldsymbol{\nu}_t) \sim \mathcal{N}_{2d}(\mathbf{0}_{2d}, C)$, with C a correlation matrix and $\mathbf{0}_{2d} = (0, \ldots, 0) \in \mathbb{R}^{2d}$.

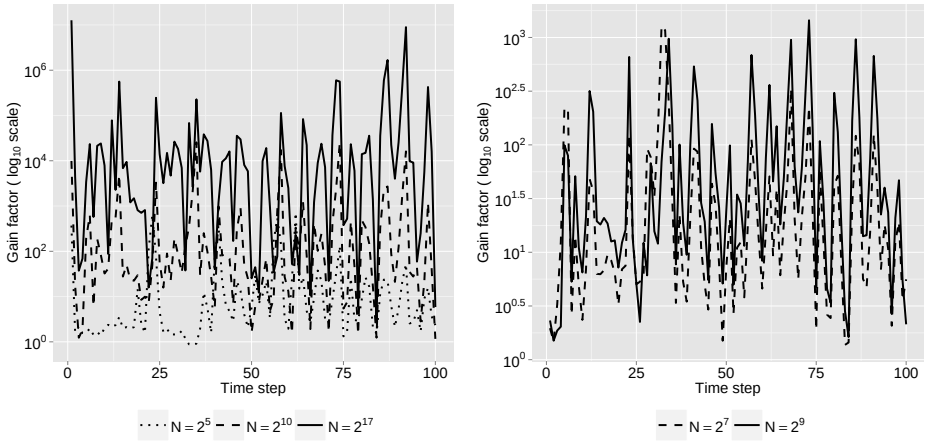

Figure 1.3: Filtering (left graph) and backward smoothing (right graph) for the toy example (1.6): gain factor as a function of t for the estimation of $\mathbb{E}[x_t|y_{0:t}]$ and for the estimation of $\mathbb{E}[x_t|y_{0:T}]$, obtained from 500 independent runs of SQMC and SMC.

In order to study the relative performance of SQMC over SMC as the dimension d of the hidden process increases we perform simulations for $d \in \{1, 2, 4, 10\}$. The parameters we use for the simulations are the same as in Chan et al. (2006): $\phi_{ii} = 0.9$, $\mu_i = -9$, $\psi_{ii}^2 = 0.1$ for all $i = 1, ..., d$ and

$$C = \begin{pmatrix} 0.6\mathbf{1}_d + 0.4\mathcal{I}_d & -0.1\mathbf{1}_d - 0.2\mathcal{I}_d \\ -0.1\mathbf{1}_d - 0.2\mathcal{I}_d & 0.8\mathbf{1}_d + 0.2\mathcal{I}_d \end{pmatrix}$$

where $\mathcal{I}_d$ is the d-dimensional identity matrix, and $\mathbf{1}_d$ is the $d \times d$ matrix having one in all its entries. Note that the errors terms $\boldsymbol{\epsilon}_t$ and $\boldsymbol{\nu}_t$ are correlated so that the weight function G_t depends now both on $\mathbf{x}_{t-1}$ and on $\mathbf{x}_t$. The prior distribution for $\mathbf{x}_0$ is the stationary distribution of the process $(\mathbf{x}_t)$ and we take $T = 399$.

The three first panels of Figure 1.5 present results for the estimation of the log-likelihood (evaluated at the true value of the parameters and for the complete dataset $y_{0:T}$), for $d \in \{1, 2, 4\}$. One sees that the gain factor increases quickly with N, and, more importantly, the MSE of SQMC converges faster than SMC even as a function of CPU time. In fact, except for a very small interval for the univariate model, SQMC always outperforms SMC in terms of MSE for the same CPU effort. We note the particularly impressive values of the gain factor we obtain for $d = 1$ when N is large: around 4.2×10^4 for $N = 2^{17}$. The last panel of Figure 1.5 plots the gain factors as a function of N, for same values of d, plus $d = 10$. The improvement brought by SQMC decreases with the dimension, and in fact, for $d = 10$, the gain factor is essentially one for the considered values of N; yet for $d = 4$ we still observe some notable improvement; e.g. a gain factor of 10 for $N \approx 10^5$. We now focus on $d = 1$, 2 and 4.

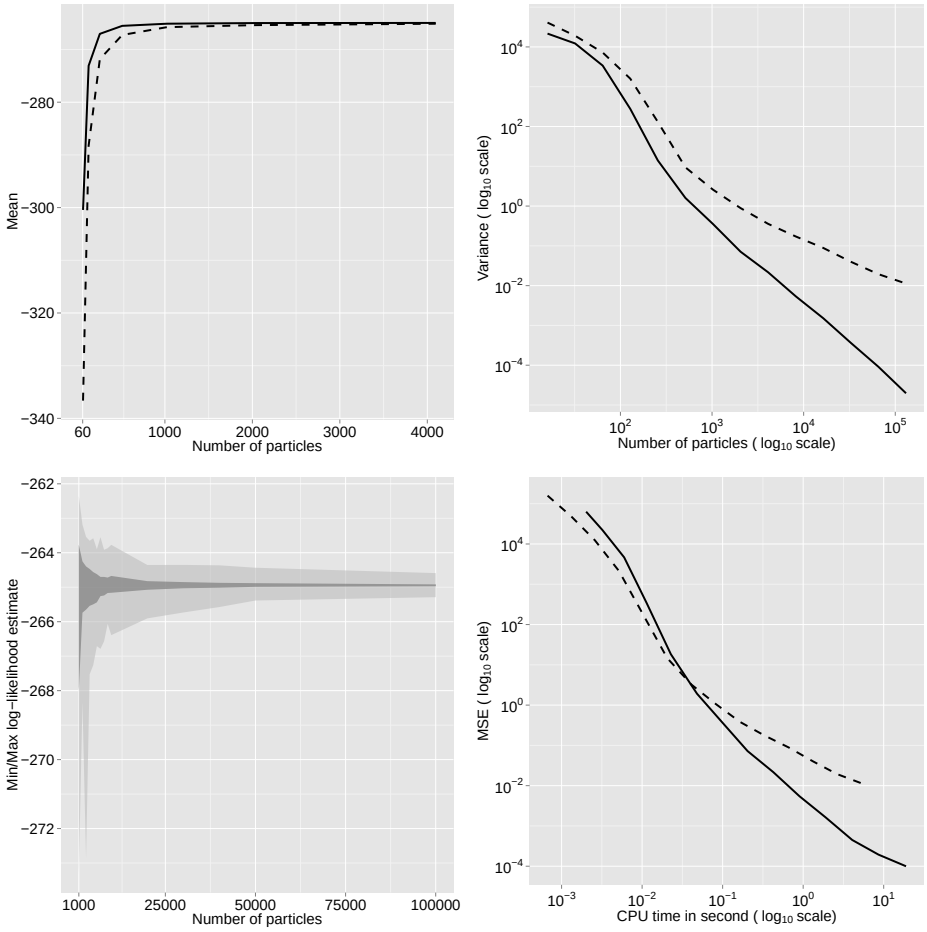

Figure 1.4: Log-likelihood estimation for the toy example (1.6). The solid lines are for SQMC while the dashed lines are for SMC. In the bottom-left graph, the dark (light) area shows the range in which lies the SQMC (SMC) estimates of the log-likelihood function. All the results are obtained from 500 independent runs of SQMC and SMC.

Figure 1.6 represents the evolution with respect to t of the MSE for the partial log-likelihood of data $y_{0:t}$ up to time t; gain factors are reported for different values of N. As we can see from these graphs, the performance of SQMC does not seem to depreciate with t.

Finally, Figure 1.7 shows that SQMC also give impressive gain when $d > 1$ concerning the estimation of the filtering expectation $\mathbb{E}[x_{1t}|\mathbf{y}_{0:t}]$ of the first component of $\mathbf{x}_t$.

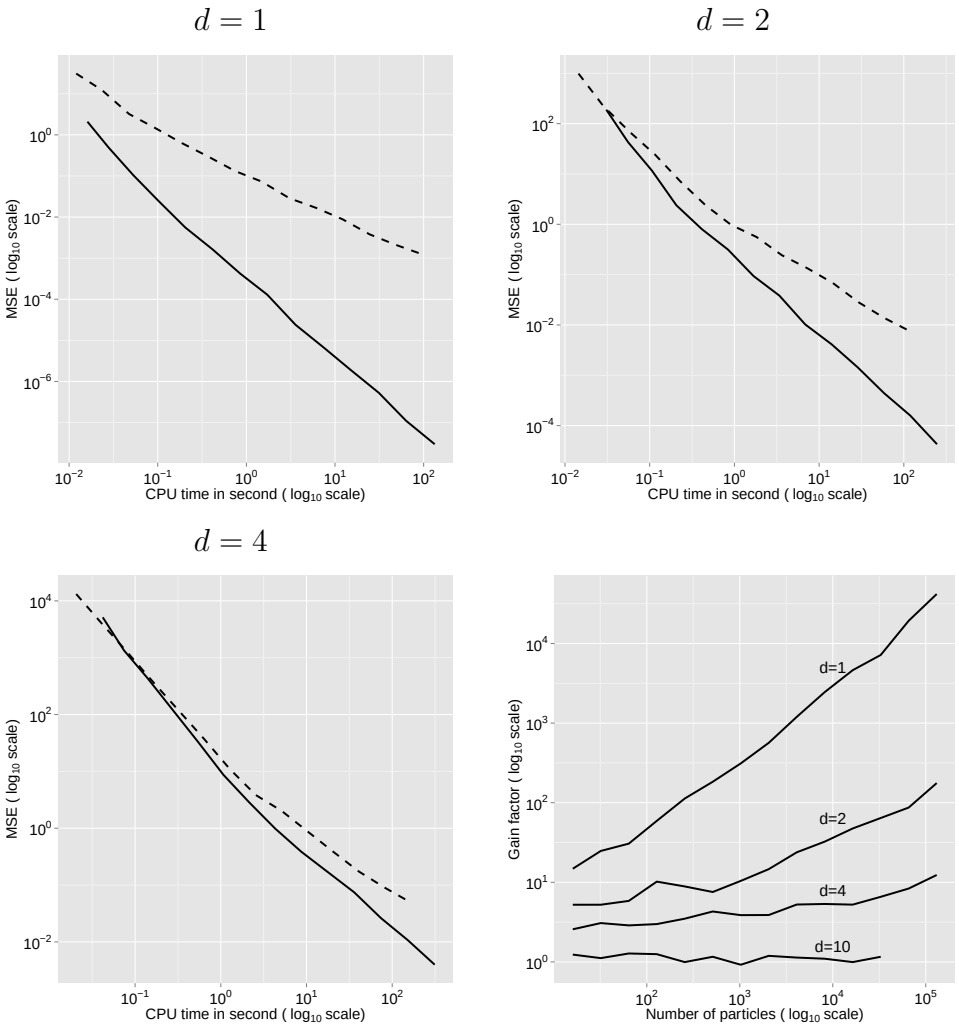

Figure 1.5: Log-likelihood estimation of SV model (1.7): MSE as a function of CPU time, for $d = 1$, 2, 4; gain factor as a function of N for $d = 1$, 2, 4 and 10. The solid lines are for SQMC while the dashed lines are for SMC. The graphs are obtained from 200 independent runs of SQMC and SMC.

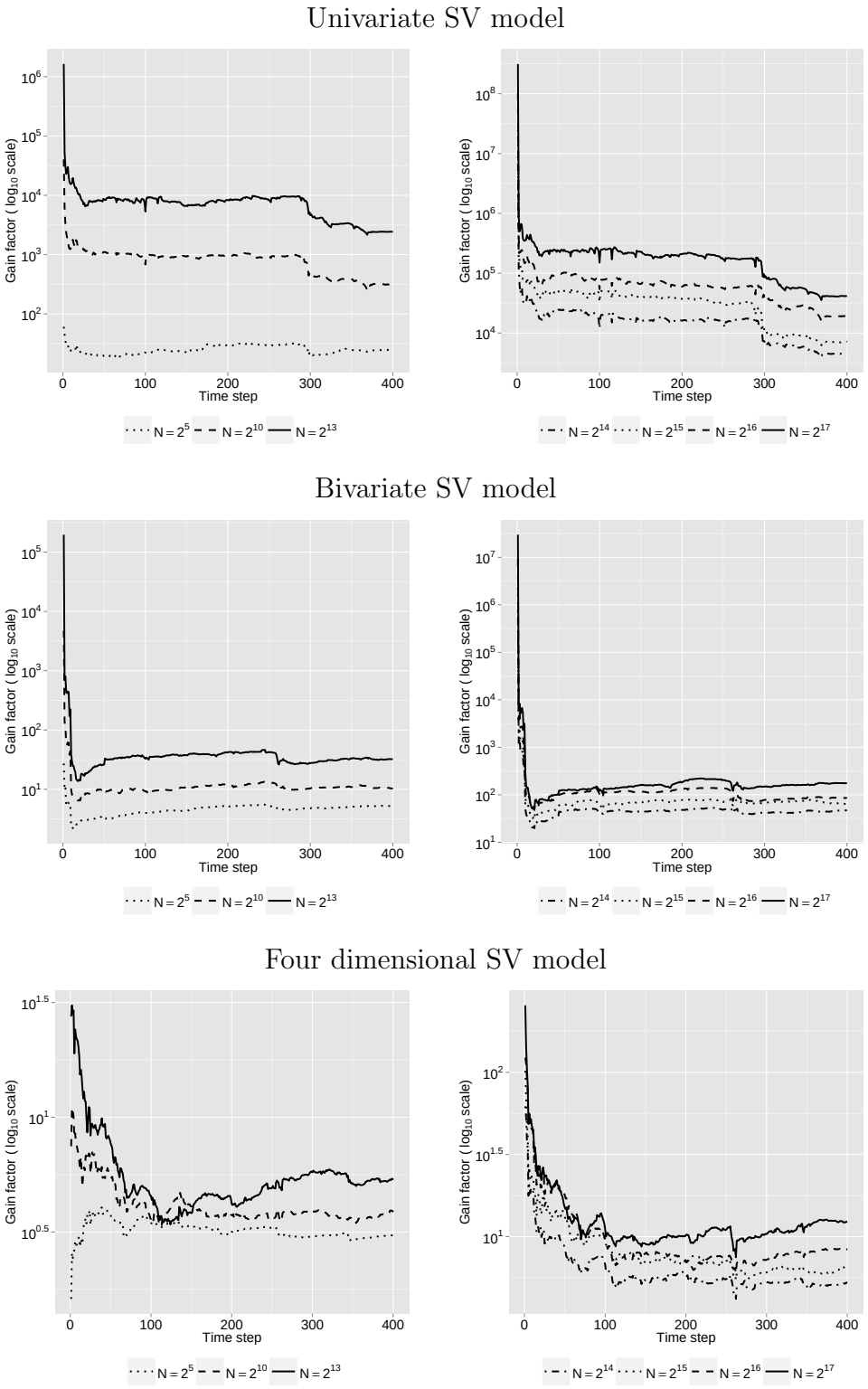

Figure 1.6: Log-likelihood estimation of the SV model (1.7): gain factor as a function of t, obtained from 200 independent runs of SQMC and SMC.

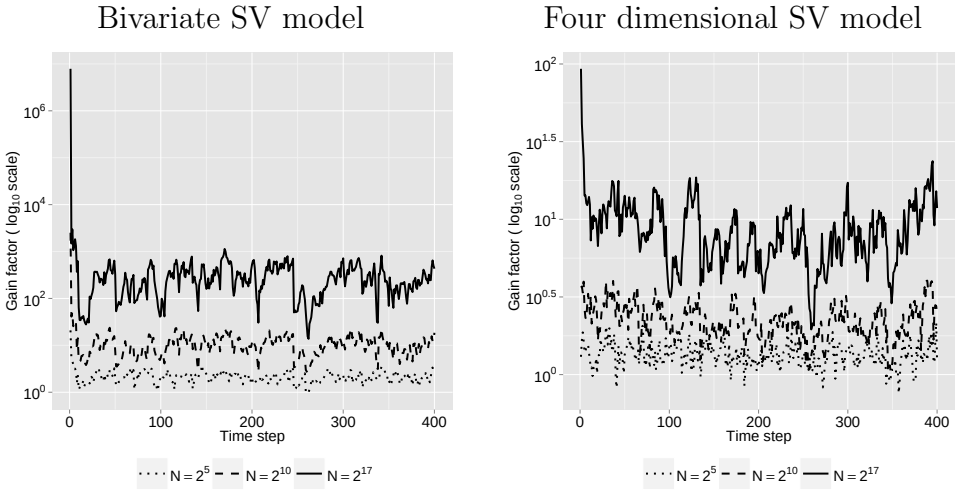

Figure 1.7: Filtering of the multivariate SV model (1.7): gain factor as a function of t for the estimation of $\mathbb{E}[x_{1t}|\mathbf{y}_{0:t}]$, obtained from 200 independent runs of SQMC and SMC.

1.5.3 Application: Bayesian estimation of MSV using PMMH on real data

To compare SMC to SQMC when used as a way to approximate the likelihood within a PMMH algorithm, as described in Section 1.4.1, we turn our attention to the Bayesian estimation of the multivariate SV model (1.7), for $d = 2$. As in Chan et al. (2006), we take the following prior:

$$\phi_{ii} \sim \mathcal{U}((0,1)), \quad 1/\psi_{ii}^2 \sim \text{Gamma}(10\exp(-10), 10\exp(-3)) \quad i = 1, \dots d,$$

where ϕ_{ii} and ψ_{ii}^2 denotes respectively the diagonal elements of Φ and Ψ, and a flat prior for $\boldsymbol{\mu}$. In addition, we assume that C is uniformly distributed on the space of correlation matrices which are such that the errors terms $\boldsymbol{\epsilon_t}$ and $\boldsymbol{\nu_t}$ are independents (no leverage effects). To sample from the posterior distribution of the parameters we use a Gaussian random walk Metropolis-Hastings algorithm with covariance matrix Σ calibrated so that the acceptance probability of the algorithm becomes, as $N \to +\infty$, close to 25%. The matrix Σ, as well as the starting point of the Markov chain, are calibrated using a pilot run of the algorithm with $\Sigma = 0.011^2\mathcal{I}_8$ and starting at the value of the parameters we used above for the simulations. To compare PMMH-SQMC with PMMH-SMC, we run the two algorithms during 10^5 iterations and for values of N ranging from 10 to 200, where N increases from 10 to 100 by increment of 10 and then by increment of 50.

We consider the following dataset: the two series are the mean-corrected daily return on the Nasdaq and S&P 500 indices for the period ranging from the 3$^{\text{rd}}$ January 2012 to the 21$^{\text{th}}$ October 2013 so that the data set contains 452 observations.

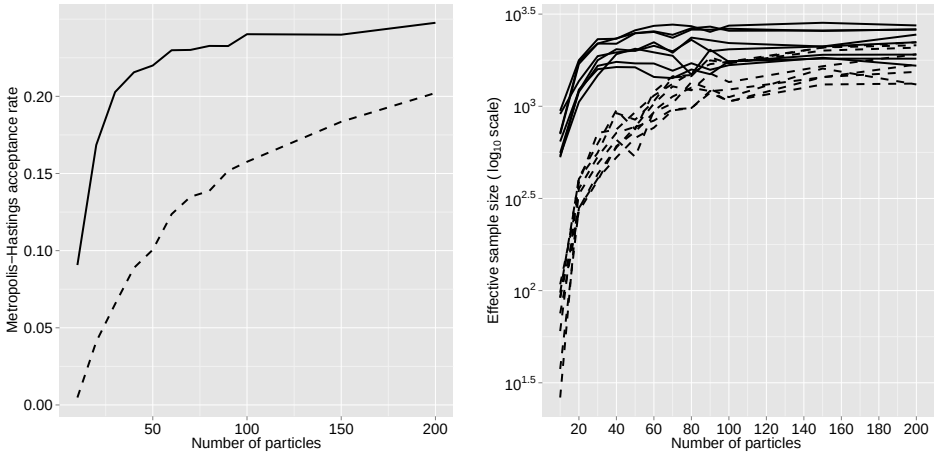

Figure 1.8: Metropolis-Hastings acceptance rate and effective sample sizes (one per parameter) for the multivariate SV model (1.7), $d = 2$, and real data: the solid lines are for PMMH-SQMC while the dashed ones are for PMMH-SMC. The results are obtained from a Markov Chain of length 10^5.

Figure 1.8 shows the Metropolis-Hastings acceptance rate and the effective sample sizes (see Robert and Casella, 2004, Section 12.3.5, for a definition) for the PMMH-SQMC algorithm and for the standard PMMH algorithm. We first observe that the acceptance rate of PMMH-SQMC increases very quickly with N. Indeed, it is already of 20% for only 30 particles while for the same number of particles the acceptance rate for the standard PMMH is approximatively 6.5%. As far as the acceptance rate is concerned, there is no significant gain to take $N > 60$ for the PMMH-SQMC algorithm while for the plain Monte Carlo algorithm the acceptance rate is only about 20% for $N = 200$ and therefore much smaller than the target of 25%. Looking at the results for the effective sample sizes (ESSs), we see that the same conclusions hold. More precisely, for the PMMH-SQMC algorithm, the ESSs increase with N much faster than for PMMH-SMC. Indeed, for $N \in 10 : 50$, the ESSs for the former is between 2.18 and 14.94 times larger than for PMMH-SMC.

1.5.4 Example 3: Neural decoding

Neural decoding models are used for brain-machine interface in order to make inference about an organism's environment from its neural activity. More precisely, we consider the problem of decoding a set of environment variables $\mathbf{p}_t \in \mathbb{R}^2$, from the firing ensemble of d_y neurons. The latent vector $\mathbf{p}_t$ may be interpreted as two-dimensional hand kinetics for motor cortical decoding (see Koyama et al., 2010, and references therein for more details about neural decoding models). Noting $\dot{\mathbf{p}}_t$ the vector of velocities, the neural decoding model we consider is given by (Koyama

et al., 2010)

$$\begin{cases} y_{ti}|\mathbf{x}_{0:t} \sim \mathcal{P}\left(\Delta \exp(\alpha_i + \beta_i^T \mathbf{x}_t)\right), & i \in 1:d_y, \qquad t \geq 0 \\ \mathbf{x}_t = \Phi \mathbf{x}_{t-1} + \Psi \boldsymbol{\epsilon}_t, & \boldsymbol{\epsilon}_t \sim \mathcal{N}_2(\mathbf{0}_2, \sigma^2 \mathcal{I}_2), \quad t > 0 \end{cases} \tag{1.8}$$

and $\mathbf{x}_0 \sim \mathcal{N}_4(\mathbf{0}_4, \mathcal{I}_4)$, where $\mathbf{x}_t = (\mathbf{p}_t, \dot{\mathbf{p}}_t)$, the y_{ti}'s are conditionally independent, $\mathcal{P}(\lambda)$ denotes the Poisson distribution with parameter λ, Δ is the duration of the interval over which spikes are counted at each time step, and

$$\Phi = \begin{pmatrix} \mathcal{I}_2 & \Delta \mathcal{I}_2 \\ \mathbf{0}_2 & \mathcal{I}_2 \end{pmatrix}, \quad \Psi^T = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Realistic values for the parameters, see Koyama et al. (2010), that we will take in ours simulations, are $d_y = 10$, $T = 23$, $\Delta = 0.03$, $\sigma^2 = 0.019$, $\alpha_i \overset{i.i.d}{\sim} \mathcal{N}_1(2.5, 1)$, $\beta_i \sim \mathcal{U}([0,1)^d)$.

One important aspect of this model is that the dimension of the noise term $\boldsymbol{\epsilon}_t$ is lower than the dimension of $\mathbf{x}_t$. As a result, two components of $\mathbf{x}_t$ are deterministic functions of $\mathbf{x}_{t-1}$. Many tracking problems have a similar structure.

This requires us to slightly adapt SQMC as follows: one samples jointly the ancestor variables $a_{t-1}^{1:N}$ and the new velocities $\dot{\mathbf{p}}_t^n$ as in Steps (b) and (c) of Algorithm 1.3, then one obtains the new $\mathbf{p}_t^n$ as $\mathbf{p}_t^n = \mathbf{p}_{t-1}^n + \dot{\mathbf{p}}_t^n$, i.e. the deterministic linear transformation of $\mathbf{p}_{t-1}^{a_{t-1}^n}$ and $\dot{\mathbf{p}}_{t-1}^n$ defined by the model. Note that in this case the dimension of the point set $\mathbf{u}_t^{1:N}$ is 3 for $t > 0$; we could say that $d = 2$ in this case, even if the dimension of $\mathbf{x}_t$ itself is 4.

Figures 1.9 and 1.10 present, respectively, results for the estimation of the log-likelihood (evaluated at the true value of the parameters) and for the estimation of the filtering expectation $\mathbb{E}[x_{ti}|\mathbf{y}_{0:t}]$ for $i \in 1:d$. Concerning the log-likelihood estimation we observe fast increase of the gain factor after about 2^{11} particles with a maximum close to 21 when N is very large. The gain of SQMC compensates its longer running time after only about 0.17 seconds. Important and increasing (in N) gains are also observed for the estimation of the filtering expectations.

1.6 Conclusion and future work

The main message of the paper is that SMC users should be strongly encouraged to switch to SQMC, as SQMC is "typically" much more accurate (produces estimates with smaller errors) than SMC. We add the word "typically" to recall that our asymptotic analysis, by construction, proves only that the SQMC error is smaller than the SMC error *for N large enough*. But our range of numerical examples, which are representative of real-world filtering problems, makes us optimistic than in most practical cases SQMC should outperform SMC even for moderate values of N.

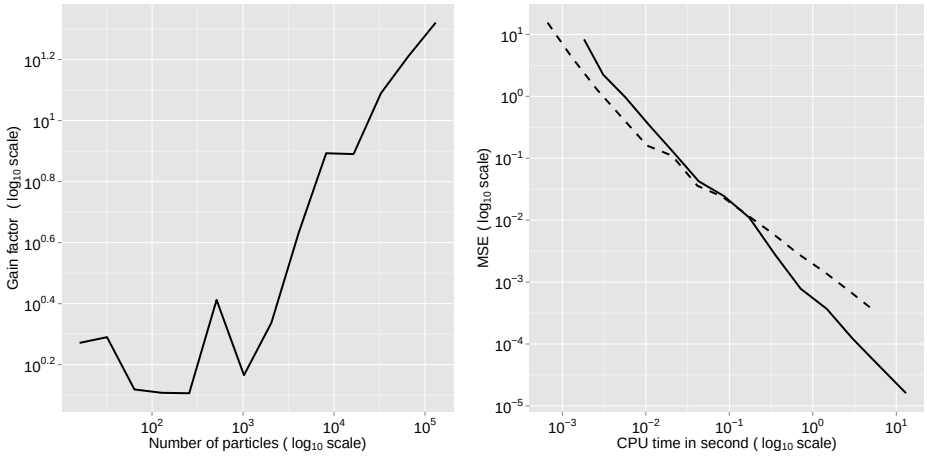

Figure 1.9: Log-likelihood estimation of the neural decoding model (1.8). The left graph gives the ratio of the SMC and the SQMC MSE. In the right graph, the solid line is for SQMC while the dashed line is for SMC. The graphs are obtained from 200 independent runs of SQMC and SMC.

The main price to pay to switch to SQMC is that users should spend some time thinking on how to write the simulation of $\mathbf{x}_t^n$ given $\mathbf{x}_{t-1}^n$ as $\mathbf{x}_t^n = \Gamma_t(\mathbf{x}_{t-1}^n, \mathbf{u}_t^n)$, where $\mathbf{u}_t^n \sim \mathcal{U}([0,1]^d)$ and Γ_t is a deterministic function that is easy to evaluate. Fortunately, this is often straightforward. In fact, there are many models of interest where $\mathbf{x}_t^n$ given $\mathbf{x}_{t-1}^n$ is linear and Gaussian. Since this case is already implemented in our program, adapting it to such a model should be just a matter of changing a few lines of code (to evaluate the probability density of $\mathbf{y}_t$ given $\mathbf{x}_t$).

Regarding future work, the most pressing tasks seem (a) to refine the convergence rate of the SQMC error; and (b) to establish that it does not degenerate over time (in the spirit of time-uniform estimates for SMC, see p. 244 of Del Moral, 2004). Regarding the former, He and Owen (2014) make the interesting conjecture that the mean square error of SQMC converges at rate $\mathcal{O}(N^{-1-2/d})$. This would explain why the relative performance of SQMC decreases with the dimension. Fortunately, a majority of the state space models of interest in signal processing, finance, or other fields are such that $d \leq 6$. A notable exception is geophysical data assimilation (in e.g. meteorology or oceanography) for which d can be very large, but for such large-dimensional problems SMC seems to perform too poorly for practical use anyway (Bocquet et al., 2010).

Finally, it is also our hope that this paper will help QMC garner wider recognition in Bayesian computation and related fields. Granted, QMC is more technical than standard Monte Carlo, and there is perhaps something specific about particle filtering that makes the introduction of QMC so effective. Yet we cannot help but think that the full potential of QMC in Statistics remains under-explored.

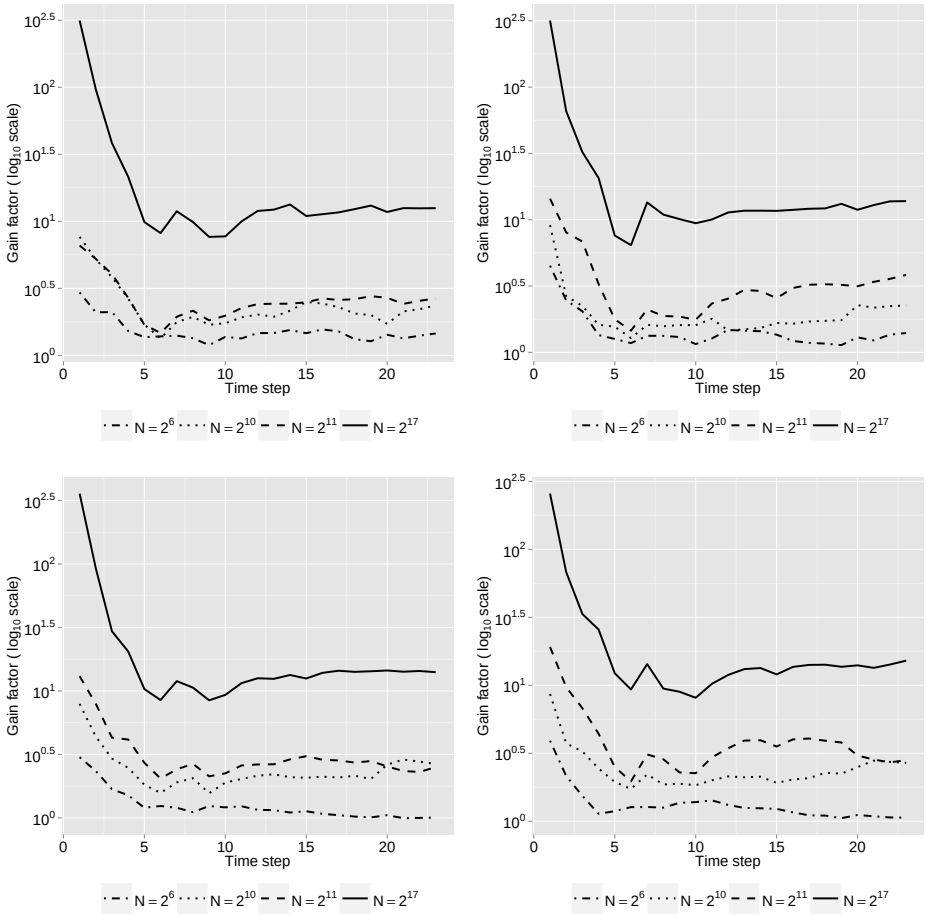

Figure 1.10: Filtering of the Neuro decoding model (1.8). From left to right and from top to bottom, the graphs give the ratio of the SMC and SQMC MSE for the estimation of $\mathbb{E}[x_{kt}|\mathbf{y}_{0:t}]$ as a function of t, $k = 1, \ldots, 4$, and are obtained from 200 independent runs of SQMC and SMC.

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Appendix: Proofs

A Importance sampling: Theorems 1.1 and 1.2

A.1 Preliminary calculation

Let $\hat{q}(\mathrm{d}\mathbf{x}) = \mathcal{S}(\mathbf{x}^{1:N})(\mathrm{d}\mathbf{x}) = N^{-1}\sum_{n=1}^{N}\delta_{\mathbf{x}^n}(\mathrm{d}\mathbf{x})$, and, as a preliminary calculation, take $\varphi \in L_2\left([0,1)^d, \lambda_d\right)$ and

$$\begin{aligned}
\left|\pi^N(\varphi) - \pi(\varphi)\right| &= \left|\frac{N^{-1}\sum_{n=1}^{N} w(\mathbf{x}^n)\varphi(\mathbf{x}^n)}{N^{-1}\sum_{n=1}^{N} w(\mathbf{x}^n)} - \pi(\varphi)\right| \\
&\leq \left|\frac{N^{-1}\sum_{n=1}^{N} w(\mathbf{x}^n)\varphi(\mathbf{x}^n)}{N^{-1}\sum_{n=1}^{N} w(\mathbf{x}^n)} - N^{-1}\sum_{n=1}^{N} w(\mathbf{x}^n)\varphi(\mathbf{x}^n)\right| \\
&\quad + \left|N^{-1}\sum_{n=1}^{N} w(\mathbf{x}^n)\varphi(\mathbf{x}^n) - q(w\varphi)\right| \\
&\leq \frac{N^{-1}\sum_{n=1}^{N} w(\mathbf{x}^n)\left|\varphi(\mathbf{x}^n)\right|}{N^{-1}\sum_{n=1}^{N} w(\mathbf{x}^n)}\left|q(w) - \hat{q}(w)\right| \\
&\quad + \left|\hat{q}(w\varphi) - q(w\varphi)\right|. \qquad (1.9)
\end{aligned}$$

We will use this inequality in the two following proofs.

A.2 Proof of Theorem 1.1

Take $\varphi = \mathbb{1}_B$ for $B \in \mathcal{B}_{[0,1)^d}$ in (1.9). Consider the first term above. The ratio is bounded by 1, and (since w is bounded) $|q(w) - \hat{q}(w)| \to 0$ by portmanteau lemma (Van der Vaart, 2007, Lemma 2.2). Now consider the second term.

We follow essentially the same steps as in Van der Vaart (2007, Lemma 2.2). Without loss of generality we assume that $q(\mathrm{d}\mathbf{x})$ is a continuous probability measure (the same argument as in Van der Vaart, 2007, is used for the general case).

Let $\epsilon > 0$ and take $J \in \mathcal{B}_{[0,1)^d}$ such that $q(J^c) \leq \epsilon$. Since J is compact, $w(\cdot)$ is uniformly continuous on J. Let $\eta > 0$ be such that $\|\mathbf{x}-\mathbf{y}\| \leq \eta \implies |w(\mathbf{x})-w(\mathbf{y})| \leq \epsilon$, $\forall(\mathbf{x},\mathbf{y}) \in J^2$. Let $\{J_k\}_{k=1}^m$ be a split of J into a finite collection of m closed

hyperrectangles with radius (at most) η. Let $g(\mathbf{x}) = \sum_{k=1}^{m} w(\mathbf{x}_k)\mathbb{I}_{J_k}(\mathbf{x})$ and note that $|w(\mathbf{x}) - g(\mathbf{x})| \leq 2^d\epsilon$, $\forall \mathbf{x} \in J$. Thus

$$\left|\int_B w(\mathbf{x})\left\{\hat{q}(\mathrm{d}\mathbf{x}) - q(\mathrm{d}\mathbf{x})\right\}\right| \leq \left|\int_B \left\{w(\mathbf{x}) - g(\mathbf{x})\right\}\hat{q}(\mathrm{d}\mathbf{x})\right| + \left|\int_B g(\mathbf{x})\left\{\hat{q}(\mathrm{d}\mathbf{x}) - q(\mathrm{d}\mathbf{x})\right\}\right| + \left|\int_B \left\{w(\mathbf{x}) - g(\mathbf{x})\right\} q(\mathrm{d}\mathbf{x})\right|$$

where for the first term we have

$$\begin{aligned}\left|\int_B (w(\mathbf{x}) - g(\mathbf{x}))\hat{q}(\mathrm{d}\mathbf{x})\right| &\leq \left|\int_{B\cap J} (w(\mathbf{x}) - g(\mathbf{x}))\hat{q}(\mathrm{d}\mathbf{x})\right| + \left|\int_{B\cap J^c} w(\mathbf{x})\hat{q}(\mathrm{d}\mathbf{x})\right| \\ &\leq 2^d\epsilon + \|w\|_\infty \hat{q}(J^c) \\ &\leq \epsilon(2^d + 2\|w\|_\infty) \end{aligned} \tag{1.10}$$

as $\hat{q}(J^c)$ converges to $q(J^c)$, and thus $\hat{q}(J^c) \leq 2\epsilon$ for N large enough; and for the second term

$$\begin{aligned}\left|\int_B g(\mathbf{x})\left\{\hat{q}(\mathrm{d}\mathbf{x}) - q(\mathrm{d}\mathbf{x})\right\}\right| &\leq \sum_{k=1}^{m} w(\mathbf{x}_k)\left|\int_{\bar{J}_k\cap B}\left\{\hat{q}(\mathrm{d}\mathbf{x}) - q(\mathrm{d}\mathbf{x})\right\}\right| \\ &\leq \|\hat{q}(\mathrm{d}\mathbf{x}) - q(\mathrm{d}\mathbf{x})\|_{\mathrm{E}} \sum_{k=1}^{m} w(\mathbf{x}_k). \end{aligned} \tag{1.11}$$

Finally, for the third term:

$$\begin{aligned}\left|\int_B \left\{w(\mathbf{x}) - g(\mathbf{x})\right\} q(\mathrm{d}\mathbf{x})\right| &\leq \left|\int_{B\cap J} \left\{w(\mathbf{x}) - g(\mathbf{x})\right\} q(\mathrm{d}\mathbf{x})\right| + \left|\int_{B\cap J^c} w(\mathbf{x})q(\mathrm{d}\mathbf{x})\right| \\ &\leq \epsilon(2^d + \|w\|_\infty). \end{aligned} \tag{1.12}$$

Putting (1.10)-(1.12) together shows that, for all $B \in \mathcal{B}_{[0,1)^d}$

$$\begin{aligned}\left|\int_B w(\mathbf{x})\left\{\hat{q}(\mathrm{d}\mathbf{x}) - q(\mathrm{d}\mathbf{x})\right\}\right| &\leq \epsilon(2^{d+1} + 3\|w\|_\infty) + \|\hat{q}(\mathrm{d}\mathbf{x}) - q(\mathrm{d}\mathbf{x})\|_{\mathrm{E}} \sum_{k=1}^{m} w(\mathbf{x}_k) \\ &\leq \epsilon(2^{d+2} + 3\|w\|_\infty) \end{aligned} \tag{1.13}$$

for N large enough (as $\|\hat{q}(\mathrm{d}\mathbf{x}) - q(\mathrm{d}\mathbf{x})\|_{\mathrm{E}} \to 0$) which concludes the proof of Theorem 1.1.

A.3 Proof of Theorem 1.2

We prove first L_1 convergence (first part of Theorem 1.2). We start again from (1.9), but for any $\varphi \in L_2\left([0,1)^d, \lambda_d\right)$. For the second term, by Jensen's inequality

$$\mathbb{E}\left|\hat{q}(w\varphi) - q(w\varphi)\right| \leq \left[\mathrm{Var}\left\{\hat{q}(w\varphi)\right\}\right]^{1/2} = \mathcal{O}(r(N)^{1/2})$$

by assumption. For the first term, using Cauchy-Schwartz, $\mathbb{E}(|CD|) \leq \{\mathbb{E}(C^2)\mathbb{E}(D^2)\}^{1/2}$ with

$$C = \frac{N^{-1}\sum_{n=1}^{N} w(\mathbf{x}^n)\,|\varphi(\mathbf{x}^n)|}{N^{-1}\sum_{n=1}^{N} w(\mathbf{x}^n)}, \quad D = q(w) - \hat{q}(w),$$

we have $\{\mathbb{E}(D^2)\}^{1/2} = \mathcal{O}(r(N)^{1/2})$, and what remains to prove is that $\mathbb{E}(C^2) = \mathcal{O}(1)$.

From (1.13), and under Assumption 2, one sees that there exists N_ϵ such that with probability one $N^{-1}\sum_{n=1}^{N} w(\mathbf{x}^n) \geq 1/2$ as soon as $N \geq N_\epsilon$. Under Assumption 1, a bound similar to (1.13) is easily obtained by replacing $\mathbf{x}^{1:N}$ with $\mathbf{u}^{1:N}$ and observing that $w \circ F_q^{-1}$ is continuous and bounded. Thus, for N large enough

$$\mathbb{E}(C^2) \leq 4\mathbb{E}\left\{\left[N^{-1}\sum_{n=1}^{N} w(\mathbf{x}^n)\,|\varphi(\mathbf{x}^n)|\right]^2\right\} \leq \mathcal{O}(r(N)) + \pi(|\varphi|)^2 = \mathcal{O}(1).$$

We now prove L_2 convergence (second part of Theorem 1.2):

$$\mathrm{Var}\left\{\pi^N(\varphi)\right\} \leq \left[\mathrm{Var}\left\{\pi^N(\varphi) - \hat{q}(w\varphi)\right\}^{1/2} + \mathrm{Var}\left\{\hat{q}(w\varphi)\right\}^{1/2}\right]^2,$$

with $\mathrm{Var}\left\{\hat{q}(w\varphi)\right\} = \mathcal{O}(r(N))$ by assumption, and for the first term:

$$\begin{aligned}
\mathbb{E}\left[\left\{\pi^N(\varphi) - \hat{q}(w\varphi)\right\}^2\right] =& \mathbb{E}\left[\left\{\sum_{n=1}^{N}\left\{W^n - N^{-1}w(\mathbf{x}^n)\right\}\varphi(\mathbf{x}^n)\right\}^2\right] \\
=& \mathbb{E}\left[\left\{1 - N^{-1}\sum_{n=1}^{N} w(\mathbf{x}^n)\right\}^2\left\{\sum_{n=1}^{N} W^n\varphi(\mathbf{x}^n)\right\}^2\right] \\
=& \mathbb{E}\left[\frac{\left\{1-\hat{q}(w)\right\}^2\hat{q}(w\varphi)^2}{\hat{q}(w)^2}\right] \\
\leq& 4\mathbb{E}\left[\left\{1-\hat{q}(w)\right\}^2\hat{q}(w\varphi)^2\right]
\end{aligned}$$

for N large enough, using the same argument as above (as $\hat{q}(w) \to 1$). Then

$$\begin{aligned}
\mathbb{E}\left[\left\{1-\hat{q}(w)\right\}^2\hat{q}(w\varphi)^2\right] \leq& \mathbb{E}\left[\left\{1-\hat{q}(w)\right\}^2\left\{\hat{q}(w\varphi) - \pi(\varphi)\right\}^2\right] - \pi(\varphi)^2\mathbb{E}\left[\left\{1-\hat{q}(w)\right\}^2\right] \\
&+ 2|\pi(\varphi)|\mathbb{E}\left[|\hat{q}(w\varphi)|\left\{1-\hat{q}(w)\right\}^2\right]
\end{aligned}$$

where for the second term, $\mathbb{E}\left[\left\{1-\hat{q}(w)\right\}^2\right] = \mathrm{Var}\left[\hat{q}(w)\right] = \mathcal{O}\left(r(N)\right)$, for the first term

$$\begin{aligned}
\mathbb{E}\left[\left\{1-\hat{q}(w)\right\}^2\left\{\hat{q}(w\varphi) - \pi(\varphi)\right\}^2\right] &= \mathbb{E}\left[\left\{1-\hat{q}(w)\right\}^2\left\{\hat{q}(w\varphi) - q(w\varphi)\right\}^2\right] \\
&\leq (1 + \|w\|_\infty)^2\mathrm{Var}\left[\hat{q}(w\varphi)\right] \\
&= \mathcal{O}\left(r(N)\right)
\end{aligned}$$

and finally for the third term

$$\mathbb{E}\left[|\hat{q}(w\varphi)|\left\{1-\hat{q}(w)\right\}^2\right] \leq \mathbb{E}\left[|\hat{q}(w\varphi)-q(w\varphi)|\left\{1-\hat{q}(w)\right\}^2\right] + |q(w\varphi)|\mathrm{Var}\left[\hat{q}(w)\right]$$

with

$$\begin{aligned}\mathbb{E}\left[|\hat{q}(w\varphi)-q(w\varphi)|\left\{1-\hat{q}(w)\right\}^2\right] &\leq (1+\|w\|_\infty)\,\mathrm{Var}\left[\hat{q}(w\varphi)\right]^{1/2}\mathrm{Var}\left[\hat{q}(w)\right]^{1/2}\\ &= \mathcal{O}\left(r(N)\right)\end{aligned}$$

which concludes the proof.

For subsequent uses (see the proof of Theorem 1.6), we note that these computations imply, for N large enough,

$$\mathrm{Var}\{\pi^N(\varphi)\} \leq \left\{2(1+\|w\|_\infty)\mathrm{Var}[\hat{q}(w\varphi)]^{1/2} + (1-2|\pi(\varphi)|)\mathrm{Var}[\hat{q}(w)]^{1/2}\right\}^2 \quad (1.14)$$

$$|\pi^N(\varphi)-\pi(\varphi)| \leq [\mathrm{Var}\{\hat{q}(w\varphi)\}]^{1/2} + 2[\mathrm{Var}\{\hat{q}(w)\}]^{1/2}\left[\mathrm{Var}\{\hat{q}(w\varphi)\} + \pi(|\varphi|)^2\right]^{1/2}. \quad (1.15)$$

B Hilbert curve and discrepancy: Theorems 1.3 and 1.4

The proofs in this Section rely on the properties of the Hilbert curved laid out in Section 1.2.3 and the corresponding notations.

B.1 Proof of Theorem 1.3

We first show that $\|\pi_h^N - \pi_h\|_{\mathrm{E}} = \sup_{0\leq a<b\leq 1}|\pi_h^N([a,b)) - \pi_h([a,b))|$. Because π_h is a continuous probability measure on $[0,1)$, the result is obvious if π_h^N is continuous as well. Let $0 \leq a < b < 1$ be such that b is a discontinuity point of $F_{\pi_h^N}$ and let $\delta > 0$ be small enough so that $\pi_h^N([a,b]) = \pi_h^N([a,b+\delta))$ and $b+\delta \leq 1$. Then,

$$\left||\pi_h^N([a,b]) - \pi_h([a,b])| - |\pi_h^N([a,b+\delta)) - \pi_h([a,b+\delta))|\right| \leq \pi_h([b,b+\delta]).$$

By the bi-measure property of the Hilbert curve, the set $H([b,b+\delta])$ has Lebesgue measure δ in $[0,1)^d$ and therefore, $\pi_h([b,b+\delta]) = \pi\big(H[b,b+\delta]\big) \leq \|\pi\|_\infty\delta$ where $\|\pi\|_\infty < +\infty$ by assumption. Hence, for all $\epsilon > 0$ small enough,

$$\left|\|\pi_h^N - \pi_h\|_{\mathrm{E}} - \sup_{0\leq a<b\leq 1}|\pi_h^N([a,b)) - \pi_h([a,b))|\right| \leq \epsilon.$$

To prove the theorem note that the above computations imply that

$$\|\pi_h^N - \pi_h\|_{\mathrm{E}} \leq 2\sup_{b\in(0,1)}|\pi_h^N([0,b]) - \pi_h([0,b])|.$$

To bound the right-hand side, let $I = [0, b]$, $b \in (0, 1)$, and $m \in \mathbb{N}$ (which may depend on N) and assume first that $b \geq 2^{-dm}$, so that $I_m^d(0) \subseteq I$. Take $\tilde{I} = [0, k^* 2^{-dm}]$, where $k^* \leq (2^{dm} - 1)$ is the largest integer such that $k^* 2^{-dm} \leq b$. Then

$$\begin{aligned}
\left|\pi_h^N(I) - \pi_h(I)\right| &\leq \left|F_{\pi_h^N}\left(k^* 2^{-dm}\right) - F_{\pi_h}\left(k^* 2^{-dm}\right)\right| \\
&\quad + \left|\pi_h^N(I) - F_{\pi_h^N}\left(k^* 2^{-dm}\right) - \left\{\pi_h(I) - F_{\pi_h}\left(k^* 2^{-dm}\right)\right\}\right| \\
&= \left|\pi^N(J) - \pi(J)\right| + \left|\pi_h^N\left((k^* 2^{-dm}, b]\right) - \pi_h\left((k^* 2^{-dm}, b]\right)\right| \quad (1.16)
\end{aligned}$$

with $J = H(\tilde{I})$. Since $\tilde{I}$ is the union of k^* intervals in $\mathcal{I}_m^d$, J is the union of k^* hypercubes in $\mathcal{S}_m^d$, and therefore (using a similar argument as above and Niederreiter, 1992, Proposition 2.4),

$$\left|\pi^N(J) - \pi(J)\right| \leq c\|\pi^N - \pi\|_{\mathrm{E}} \leq 2^{dm} r(N)$$

for a constant c and where $r(N) = \|\pi^N - \pi\|_{\mathrm{E}}$.

For the second term of (1.16), by the properties of the Hilbert curve,

$$\begin{aligned}
\left|\pi_h^N\left((k 2^{-dm}, b]\right) - \pi_h\left((k 2^{-dm}, b]\right)\right| &\leq \pi_h^N\left(I_m^d(k)\right) + \pi_h\left(I_m^d(k)\right) \\
&= \pi^N\left(S_m^d(k)\right) + \pi\left(S_m^d(k)\right) \\
&\leq 2\pi\left(S_m^d(k)\right) + r(N) \\
&= \mathcal{O}\left(2^{-dm} \vee r(N)\right)
\end{aligned}$$

where the last inequality comes from the fact that $\pi(\mathbf{x})$ is a bounded density.

In case $b < 2^{-dm}$, similar computations show that

$$\left|\pi_h^N(I) - \pi_h(I)\right| \leq \pi_h^N(I_m^d(0)) + \pi_h(I_m^d(0)) = \mathcal{O}\left(2^{-dm} \vee r(N)\right).$$

To conclude, we choose m so that $2^{-dm} = \mathcal{O}(r(N)^{1/2})$, which gives

$$\sup_{b \in (0,1)} \left|\pi_h^N([0, b]) - \pi_h([0, b])\right| = \mathcal{O}\left(r(N)^{1/2}\right).$$

Finally, since replacing $[0, b]$ by $[0, a)$ changes nothing to the proof of the result above, one may conclude that $\sup_{I \in \mathcal{B}_{[0,1)}} |\pi_h^N(I) - \pi_h(I)| = \mathcal{O}(r(N)^{1/2})$.

B.2 Proof of Theorem 1.4

Preliminary computations

The proof of this result is based on Hlawka and Mück (1972, "Satz 2"). Compared to this latter, the main technical difficulty comes from the fact that the Rosenblatt transformation $F_{\pi_h^N \otimes K_h}$ is not continuous because π_h^N is a weighted sum of Dirac measures. To control the "jumps" of the inverse Rosenblatt transformation $F^{-1}_{\pi_h^N \otimes K_h}$ introduced by the discontinuity of π_h^N, we first prove the following Lemma.

Lemma 1.1. *Consider the set-up of Theorem 1.4. For $n \in 1:N$, let $h_1^n = H(\mathbf{x}_1^n)$ and assume that the points $h_1^{1:N}$ are labelled so that $n < m \implies h_1^n < h_1^m$. (Note that the inequality is strict because, by Assumption 2 of Theorem 1.4, the points $\mathbf{x}^{1:N}$ are distinct.) Without loss of generality, assume that $h_1^1 > 0$ and let $h_1^0 = 0$. Then, as $N \to +\infty$,*

$$\max_{n \in 1:N} |h_1^n - h_1^{n-1}| \to 0.$$

To prove this Lemma, let $J_N = [h_1^{n^*-1}, h_1^{n^*}]$ where $|h_1^{n^*} - h_1^{n^*-1}| = \max_{n \in 1:N} |h_1^n - h_1^{n-1}|$. Since J_N contains at most two points, we have

$$\pi_h(J_N) \leq \pi_h^N(J_N) + r_2(N) \leq 2r_1(N) + r_2(N)$$

where $r_1(N) = \max_{n \in 1:N} W_N^n$ and $r_2(N) = \|\pi_h^N - \pi_h\|_{\mathrm{E}}$; note $r_1(N) \to 0$ by Assumption 2 of Theorem 1.4 while $r_2(N) \to 0$ by Assumption 3 of Theorem 1.4 and by Theorem 1.3. Therefore, $\pi_h(J_N) \to 0$ as $N \to +\infty$.

Assume now that $\max_{n \in 1:N} |h_1^n - h_1^{n-1}| \not\to 0$. Then, this means that there exists a $\epsilon \in (0,1)$ such that, for all $N > 1$ there exists a $N^* \geq N$ for which $\lambda_1(J_{N^*}) \geq \epsilon$. Assume first that $J_{N^*} \subset [0, 1 - \frac{\epsilon}{2}]$. In that case, we have $\pi_h(J_{N^*}) \geq c_\epsilon$ for a constant $c_\epsilon > 0$. Indeed, by the continuity of the Hilbert curve, the set $H([0, 1-\frac{\epsilon}{2}])$ is compact and therefore, $\forall \mathbf{x} \in H([0, 1 - \frac{\epsilon}{2}])$, $\pi(\mathbf{x}) \geq \underline{\pi}^{(\epsilon)}$ for a constant $\underline{\pi}^{(\epsilon)} > 0$ because the density $\pi(\mathbf{x})$ is continuous and strictly positive. Therefore, if $J_{N^*} \subset [0, 1 - \frac{\epsilon}{2}]$, we have

$$\pi_h(J_{N^*}) = \pi(H(J_{N^*})) \geq \underline{\pi}^{(\epsilon)} \lambda_d(H(J_{N^*})) = \underline{\pi}^{(\epsilon)} \lambda_1(J_{N^*}) \geq \epsilon \underline{\pi}^{(\epsilon)}$$

where the second equality uses the bi-measure property of the Hilbert curve.

Assume now that $J_{N^*} \not\subset [0, 1 - \frac{\epsilon}{2}]$. Write $J_{N^*} = [a_{N^*}, b_{N^*}]$ and note that, since $\lambda_1(J_{N^*}) \geq \epsilon$, we have $a_n^* < 1 - \epsilon$ and therefore

$$\pi_h(J_{N^*}) = \pi_h\left(\left[a_{N^*}, 1 - \frac{\epsilon}{2}\right]\right) + \pi_h\left(\left(1 - \frac{\epsilon}{2}, b_{N^*}\right]\right) \geq \left(1 - \frac{\epsilon}{2} - a_{N^*}\right) \underline{\pi}^{(\epsilon)} \geq \frac{\epsilon}{2} \underline{\pi}^{(\epsilon)}.$$

Thus, this shows that if $\max_{n \in 1:N} |h_1^n - h_1^{n-1}| \not\to 0$, then there exists a $\epsilon \in [0,1)$ such that $\limsup_{N \to +\infty} \pi_h(J_N) \geq (\epsilon \underline{\pi}^{(\epsilon)})/2 > 0$. This contradicts the fact that $\pi_h(J_N) \to 0$ as $N \to +\infty$ and the proof is complete.

Proof of Theorem 1.4

We use the shorthand $\alpha_N(B) = \mathcal{S}(\mathbf{u}^{1:N})(B)$ for any set $B \subset [0,1)^{1+d_2}$. One has

$$\|\mathcal{S}(P_h^N) - \pi_h^N \otimes K_h\|_{\mathrm{E}} = \sup_{B \in \mathcal{B}^N_{[0,1)^{1+d_2}}} \left|\alpha_N\left(E^N(B)\right) - \lambda_{1+d_2}\left(E^N(B)\right)\right|$$

where

$$\mathcal{B}^N_{[0,1)^{1+d_2}} = \left\{ B = [\boldsymbol{a}, \boldsymbol{b}] \in \mathcal{B}_{[0,1)^{1+d_2}} : \min_{n \in 1:N} h(\mathbf{x}_1^n) \leq F_{\pi_h^N}(b_1) \leq \max_{n \in 1:N} h(\mathbf{x}_1^n) \right\},$$

and where, for an arbitrary set $\tilde{B} = [a_1, b_1] \times [\boldsymbol{a}', \boldsymbol{b}']$ with $0 \leq a_1 \leq b_1 < 1$ and with $0 \leq a'_i \leq b'_i < 1$ for all $i \in 1 : d_2$, we use the shorthand $E^N(\tilde{B})$ for the set

$$\left\{(u_1, \mathbf{u}_2) \in [0,1)^{1+d_2} : F_{\pi_h^N}(a_1) \leq u_1 \leq F_{\pi_h^N}(b_1), \mathbf{u}_2 \in F_{K_h}\left(F^{-1}_{\pi_h^N}(u_1), [\boldsymbol{a}', \boldsymbol{b}']\right)\right\}.$$

Let $\mathcal{P}$ be a partition of $[0,1)^{1+d_2}$ in $L^{d_1+d_2}$ congruent hyperrectanges W of size $L^{-d_1} \times L^{-1} \times ... \times L^{-1}$ where $L \geq 1$ is an arbitrary integer. Let $B = [a_1, b_1] \times [\boldsymbol{a}', \boldsymbol{b}'] \in \mathcal{B}^N_{[0,1)^{1+d_2}}$, $\mathcal{U}_1$ the set of the elements of $\mathcal{P}$ that are strictly in $E^N(B)$, $\mathcal{U}_2$ the set of elements $W \in \mathcal{P}$ such that $W \cap \partial(E^N(B)) \neq \varnothing$, $U_1 = \cup\, \mathcal{U}_1$, $U_2 = \cup\, \mathcal{U}_2$, and $U'_1 = E^N(B) \setminus U_1$ so that

$$\alpha_N\left(E^N(B)\right) - \lambda_{1+d_2}\left(E^N(B)\right) = \alpha_N(U_1) - \lambda_{1+d_2}(U_1) + \alpha_N(U'_1) - \lambda_{1+d_2}(U'_1).$$

To bound $\alpha_N(U'_1) - \lambda_{1+d_2}(U'_1)$, note that we can cover U'_1 with sets in $\mathcal{U}_2$, hence

$$\alpha_N(U'_1) - \lambda_{1+d_2}(U'_1) \leq \alpha_N(U_2), \quad \text{and } \alpha_N(U'_1) - \lambda_{1+d_2}(U'_1) \geq -\lambda_{1+d_2}(U_2)$$

so that, by the definition of $D(\mathbf{u}^{1:N})$,

$$\begin{aligned} |\alpha_N(U'_1) - \lambda_{1+d_2}(U'_1)| &\leq |\alpha_N(U_2) - \lambda_{1+d_2}(U_2)| + \lambda_{1+d_2}(U_2) \\ &\leq \#\mathcal{U}_2 \left\{D(\mathbf{u}^{1:N}) + L^{-(d_1+d_2)}\right\}. \end{aligned}$$

We therefore have

$$\begin{aligned} \left|\alpha_N\left(E^N(B)\right) - \lambda_{1+d_2}\left(E^N(B)\right)\right| &\leq |\alpha_N(U_1) - \lambda_{1+d_2}(U_1)| + \#\mathcal{U}_2 \left\{D(\mathbf{u}^{1:N}) + L^{-(d_1+d_2)}\right\} \\ &\leq L^{d_1+d_2} D(\mathbf{u}^{1:N}) + \#\mathcal{U}_2 \left\{D(\mathbf{u}^{1:N}) + L^{-(d_1+d_2)}\right\}. \end{aligned}$$

The rest of the proof is dedicated to bounding $\#\mathcal{U}_2$, the number of hyperrectangles in $\mathcal{P}$ required to cover $\partial\left(E^N(B)\right)$. To that effect, first note that, using the continuity of F_{K_h} and the fact that B and $E^N(B)$ are closed sets, we can easily show that $E^N(\partial(B)) \subset \partial(E^N(B))$. Let $\#\mathcal{U}_2^{(1)}$ and $\#\mathcal{U}_2^{(2)}$ be, respectively, the number of hyperrectangles in $\mathcal{P}$ we need to cover $E^N(\partial(B))$ and to cover $P(B) := \partial(E^N(B)) \setminus E^N(\partial(B))$. Hence, $\#\mathcal{U}_2 \leq \#\mathcal{U}_2^{(1)} + \#\mathcal{U}_2^{(2)}$ and we now bound $\#\mathcal{U}_2^{(i)}$, $i \in 1 : 2$.

To bound $\#\mathcal{U}_2^{(1)}$ we first cover $\partial(B)$ with hyperrectangles belonging to a partition $\mathcal{P}'$ of the set $[0,1)^{1+d_2}$. We construct $\mathcal{P}'$ as a partition of the set $[0,1)^{1+d_2}$ into hyperrectangles W' of size $L'^{-d_1} \times L'^{-1} \times ... \times L'^{-1}$ such that, for all points $(h_1, \mathbf{x}_2)$ and $(h'_1, \mathbf{x}'_2)$ in W', we have

$$\left\|F_{K_h}(h_1, \mathbf{x}_2) - F_{K_h}(h'_1, \mathbf{x}'_2)\right\|_\infty = \left\|F_K(H(h_1), \mathbf{x}_2) - F_K(H(h'_1), \mathbf{x}'_2)\right\|_\infty \leq L^{-1} \tag{1.17}$$

and

$$|F_{\pi_h^N}(h_1) - F_{\pi_h^N}(h'_1)| \leq L^{-d_1}. \tag{1.18}$$

Let $L' = 2^m$ for an integer $m \geq 0$, so that h_1 and h_1' are in the same interval $I_m^{d_1}(k) \in \mathcal{I}_m^{d_1}$, and $H(h_1)$ and $H(h_1')$ belong to the same hypercube in $\mathcal{S}_m^{d_1}$. Let C_K be the Lipschitz constant of F_K, then

$$\begin{aligned}\|F_K\left(H(h_1), \mathbf{x}_2\right) - F_K\left(H(h_1'), \mathbf{x}_2'\right)\|_\infty &\leq C_K \left\{\|\mathbf{x}_2 - \mathbf{x}_2'\|_\infty \vee \|H(h_1) - H(h_1')\|_\infty\right\} \\ &\leq C_K L'^{-1}\end{aligned}$$

and Condition (1.17) is verified as soon as $L' \geq C_K L$. Let us now look at Condition (1.18). We have:

$$\begin{aligned}\left|F_{\pi_h^N}(h_1) - F_{\pi_h^N}(h_1')\right| &\leq 2\|F_{\pi_h^N} - F_{\pi_h}\|_\infty + |F_{\pi_h}(h_1) - F_{\pi_h}(h_1')| \\ &\leq 2r_2(N) + |F_{\pi_h}(h_1) - F_{\pi_h}(h_1')|\end{aligned}$$

where, as in the proof of Lemma 1.1, $r_2(N) = \|\pi_h^N - \pi_h\|_{\mathrm{E}}$. Since h_1 and h_1' are in the same interval $I_m^{d_1}(k) \in \mathcal{I}_m^{d_1}$,

$$|F_{\pi_h}(h_1) - F_{\pi_h}(h_1')| \leq \pi_h\left(I_m^{d_1}(k)\right) = \pi\left(S_m^{d_1}(k)\right) \leq \frac{\|\pi\|_\infty}{(L')^{d_1}}$$

as π is bounded. To obtain both (1.17) and (1.18), we can take $L' = 2^m$ to be the smallest power of 2 such that $L' \geq k_N L$ where

$$k_N = C_K + \left(\frac{\|\pi\|_\infty}{(1 - L^{d_1} 2r_2(N))}\right)^{1/d_1}$$

which implies that we assume from now on that $L^{-d_1} \geq 4r_2(N)$ for N large enough.

Let $R \in \partial B$ be a d_2-dimensional face of B and let $\mathcal{R}$ be the set of hyperrectangles $W' \in \mathcal{P}'$ such that $R \cap W' \neq \varnothing$. Note that $\#\mathcal{R} \leq L'^{d_1+d_2-1} \leq (2k_N L)^{d_1+d_2-1}$. For each $W' \in \mathcal{R}$, take a point $\mathbf{r}^{W'} = (r_1^{W'}, \mathbf{r}_2^{W'}) \in R \cap W'$ and define

$$\tilde{\mathbf{r}}^{W'} = (\tilde{r}_1^{W'}, \tilde{\mathbf{r}}_2^{W'}) = F_{\pi_h^N \otimes K_h}(\mathbf{r}^{W'}) \in E^N(R).$$

Let $\tilde{\mathcal{R}}$ be the collection of hyperrectangles $\tilde{W}$ of size $4L^{-d_1} \times 2L^{-1} \times ... \times 2L^{-1}$ and having point $\tilde{\mathbf{r}}^{W'}$, $W' \in \mathcal{R}$, as middle point.

For an arbitrary $\mathbf{u} = (u_1, \mathbf{u}_2) \in E^N(R)$, let $h_1 = a_1 \vee F_{\pi_h^N}^{-1}(u_1)$ and $\mathbf{x}_2 = F_{K_h}^{-1}(h_1, \mathbf{u}_2)$. Since $\mathbf{x} = (h_1, \mathbf{x}_2) \in R$, $\mathbf{x}$ is in one hyperrectangle $W' \in \mathcal{R}$. Hence, using (1.17) and (1.18),

$$|u_1 - \tilde{r}_1^{W'}| \leq |F_{\pi_h^N}(h_1) - F_{\pi_h^N}(r_1^{W'})| + |u_1 - F_{\pi_h^N}(h_1)| \leq L^{-d_1} + r_1(N),$$

where, as in the proof of Lemma 1.1, $r_1(N) = \max_{n \in 1:N} W_N^n$, and

$$\|\mathbf{u}_2 - \tilde{\mathbf{r}}_2^{W'}\|_\infty = \|F_{K_h}\left(h_1, \mathbf{x}_2\right) - F_{K_h}(r_1^{W'}, \mathbf{r}_2^{W'})\|_\infty \leq L^{-1}.$$

Assume from now on that $L^{-d_1} \geq r_1(N) + 4r_2(N)$. Then, this shows that $\mathbf{u}$ belongs to the hyperrectangle $\tilde{W} \in \tilde{\mathcal{R}}$ with center $\tilde{\mathbf{r}}^{W'}$ so that $E^N(R)$ is covered by at most $\#\tilde{\mathcal{R}} = \#\mathcal{R} \leq (2k_N L)^{d_1+d_2-1}$ hyperrectangles $\tilde{W} \in \tilde{\mathcal{R}}$. To go back to the initial partition of $[0,1)^{1+d_2}$ with hyperrectangles in $\mathcal{P}$, remark that every hyperrectangles in $\tilde{\mathcal{R}}$ is covered by at most c^* hyperrectangles in $\mathcal{P}$ for a constant c^*. Finally, since the set ∂B is made of the union of $2(d_2+1)$ d_2-dimensional faces of B, we have

$$\#\mathcal{U}_2^{(1)} \leq c_N L^{d_1+d_2-1} \tag{1.19}$$

where $c_N = c^* 2(d_2+1)(2k_N)^{d_1+d_2-1}$.

We now consider the problem of bounding $\#\mathcal{U}_2^{(2)}$, the number of hyperrectangles in $\mathcal{P}$ we need to cover the set $P(B) = \partial(E^N(B)) \setminus E^N(\partial(B))$. Note that $P(B)$ contains the boundaries of the set $E^N(B)$ that are due to the discontinuities of $F_{\pi_h^N \otimes K_h}$.

To that effect, we show that there exists a finite collection $\{D_m^N\}_{m=1}^k$ of sets in $\mathcal{B}^N_{[0,1)^{1+d_2}}$ such that, for any $\mathbf{u} = (u_1, \mathbf{u}_2) \in P(B)$, there exists a $m^* \in 1:k$ and a point $\tilde{\mathbf{u}} = (\tilde{u}_1, \tilde{\mathbf{u}}_2) \in E^N(\partial(D^N_{m^*}))$ which verifies $\tilde{u}_1 = u_1$ and $\|\mathbf{u}_2 - \tilde{\mathbf{u}}_2\|_\infty \leq C r_3(N)^{1/d_1}$ for a constant C and where $r_3(N) = \max_{n \in 1:N} |h_1^n - h_1^{n-1}|$; note that $r_3(N) \to 0$ as $N \to +\infty$ by Lemma 1.1. Hence, by taking L small enough (i.e. such that $L^{-1} \geq 2C r_3(N)^{1/d_1}$), we have $\#\mathcal{U}_2^{(2)} \leq \sum_{m=1}^k \#\mathcal{U}_2^{(D_m^N)}$ where $\#\mathcal{U}_2^{(D_m^N)}$ is the number of hyperrectangles in $\mathcal{P}$ we need to cover $E^N(\partial(D_m^N))$. Then, because the bound we derived above for the number of these hyperrectangles required to cover $E^N(\partial(B)))$ is uniform in $B \in \mathcal{B}^N_{[0,1)^{1+d_2}}$, one can conclude using (1.19) that $\mathcal{U}_2^{(2)} \leq k c_N L^{d_1+d_2-1}$.

To construct the collection $\{D_m^N\}_{m=1}^k$, let $\mathbf{u} = (u_1, \mathbf{u}_2) \in P(B)$, that is, $u_1 = F_{\pi_h^N}(h_1^{n^*})$ for a $n^* \in 1:N$ and $\mathbf{u}_2 = F_{K_h}(h_1^{n^*}, \mathbf{x}^*)$ with $\mathbf{x}^* \in (\boldsymbol{a}', \boldsymbol{b}')$. By the definition of the boundary of a set, for any $\epsilon > 0$ there exists a $\mathbf{v} = (v_1, \mathbf{v}_2) \notin E^N(B)$ such that $\|\mathbf{u} - \mathbf{v}\|_\infty \leq \epsilon$. Let $\epsilon > 0$ and assume that the point $\mathbf{v} = (u_1 - \epsilon, \mathbf{u}_2)$ verifies this condition, that is, $\mathbf{u}_2 \notin F_{K_h}(h_1^{n^*-1}, [\boldsymbol{a}', \boldsymbol{b}'])$, $n^* > 1$. (The case $v_1 = (u_1 + \epsilon, \mathbf{u}_2)$ is treated in a similar way, just replace $n^* - 1$ by $n^* + 1$ in what follows.)

We now show that there exists a set $B^N \in \mathcal{B}^N_{[0,1)^{1+d_2}}$ and a point $\tilde{\mathbf{u}} = (u_1, \tilde{\mathbf{u}}_2) \in E^N(\partial(B^N))$ such that $\|\mathbf{u}_2 - \tilde{\mathbf{u}}_2\|_\infty \leq C r_3(N)^{1/d_1}$ for a constant C. We consider the set $B^N = [a_1, b_1] \times [\boldsymbol{a}^N, \boldsymbol{b}^N]$ where $\boldsymbol{a}^N < \boldsymbol{b}^N \in [0,1)^{d_2}$. In order to construct $[\boldsymbol{a}^N, \boldsymbol{b}^N]$, we write $F_i(h_1, x_{1:i-1}, x_i)$ the i-th coordinate of $F_{K_h}(h_1, \mathbf{x})$ (with the natural convention $F_i(h_1, x_{1:i-1}, x_i) = F_1(h_1, x_1)$ when $i = 1$).

Let i^* be smallest index $i \in 1:d_2$ such that $u_{2i} \neq F_i(h_1^{n^*-1}, x_{1:i-1}, x_i)$, $\forall \mathbf{x} \in [\boldsymbol{a}', \boldsymbol{b}']$. Then, for $i \in 1:(i^*-1)$, set $\tilde{u}_{2i} = u_{2i}$ and $\tilde{x}_i = x_i^*$, while, for $i \in 1:i^*$, we set $a_i^N = a_i'$ and $b_i^N = b_i'$.

To choose $\tilde{u}_{2i^*}$ and $\tilde{x}_{i^*}$ we proceed as follows: if $F_{i^*}(h_1^{n^*-1}, x^*_{1:i^*-1}, b'_{i^*}) < u_{2i^*}$, we take $\tilde{u}_{2i^*} = F_{i^*}(h_1^{n^*}, x^*_{1:i^*-1}, b'_{i^*})$ and $\tilde{x}_{i^*} = b'_{i^*}$ so that, noting C_H the Hölder constant of H,

$$0 \leq \tilde{u}_{2i^*} - u_{2i^*} \leq F_{i^*}(h_1^{n^*}, x^*_{1:i^*-1}, b'_{i^*}) - F_{i^*}(h_1^{n^*-1}, x^*_{1:i^*-1}, b'_{i^*}) \leq C_K C_H r_3(N)^{1/d_1}$$

as required; if $F_{i^*}(h_1^{n^*-1}, x^*_{1:i^*-1}, a'_{i^*}) > u_{2i^*}$, we take $\tilde{u}_{2i^*} = F_{i^*}(h_1^{n^*}, x^*_{1:i^*-1}, a'_{i^*})$ and $\tilde{x}_{i^*} = a'_{i^*}$ so that

$$0 \leq u_{2i^*} - \tilde{u}_{2i^*} \leq F_{i^*}(h_1^{n^*-1}, x^*_{1:i^*-1}, a'_{i^*}) - F_{i^*}(h_1^{n^*}, x^*_{1:i^*-1}, a'_{i^*}) \leq C_K C_H r_3(N)^{1/d_1}$$

as required.

Then, for $i \in (i^*+1) : d_2$, take $\tilde{u}_{2i} = u_{2i}$ and $a_i^N = 0$. Finally, to construct the right boundaries b_i^N, $i \in (i^*+1) : d_2$, we define

$$u^*_{2i} = \max_{n \in 1:N} \left\{ \sup \left\{ v \in F_i \left(h_1^n, [0, b'_{1:i}] \right) \right\} \right\}, \quad i = 1, \dots d_2.$$

Note that $u^*_{2i} \in (0,1)$ for all $i \in 1 : d_2$. Indeed, the continuity of F_i and the fact that $[0, b'_{1:i}]$ is compact imply that

$$v_i^n := \sup \left\{ v \in F_i \left(h_1^n, [0, b'_{1:i}] \right) \right\} \in F_i \left(h_1^n, [0, b'_{1:i}] \right).$$

Then, since $b'_i \in (0,1)$ and F_i is strictly increasing with respect to its i-th coordinate on $[0,1)$, we indeed have $v_i^n \in (0,1)$ for all $n \in 1 : N$.

The right boundaries b_i^N, $i \in (i^*+1) : d_2$ are then defined recursively as follows:

$$b_i^N = \inf \left\{ c \in [0,1], g_i(c) \geq u^*_{2i} \right\}, \quad i = i^*+1, \dots, d_2$$

where

$$g_i(c) = \min_{(h_1, x_{1:i-1}) \in [a_1, b_1] \times [a^N_{1:i-1}, b^N_{1:i-1}]} \tilde{F}_i(h_1, x_{1:i-1}, c),$$

with $\tilde{F}_i(\cdot)$ the continuous extension of $F_i(\cdot)$ on $[0,1]^{i+1}$. (Note that such an extension exists because F_i is Lipschitz.) Because $\tilde{F}_i(h_1, x_{1:i-1}, c)$ is continuous in $(h_1, x_{1:i-1}, c)$ and $[a_1, b_1] \times [a^N_{1:i-1}, b^N_{1:i-1}] \times [0,1]$ is compact, the function g_i is continuous on $[0,1]$ with $g_i(0) = 0$ and $g_i(1) = 1$. Therefore, as $u^*_{2i} \in (0,1)$, we indeed have $b_i^N \in (0,1)$ for all $i \in (i^*+1) : d_2$, as required.

To show that $\tilde{\mathbf{u}} = (u_1, \tilde{\mathbf{u}}_2) \in E^N(\partial(B^N))$, note that, by the construction of $\boldsymbol{b}^N$ we have, for all $i \in (i^*+1) : d_2$,

$$F_i(h_1, x_{1:i-1}, b_i^N) \geq u^*_{2i} \geq u_{2i}, \quad \forall (h_1, x_{1:i-1}) \in [a_1, b_1] \times [a^N_{1:i-1}, b^N_{1:i-1}].$$

Therefore, by the continuity of F_i, for any $(h_1, x_{1:i-1}) \in [a_1, b_1] \times [a^N_{1:i-1}, b^N_{1:i-1}]$ there exists a $x_i \leq b_i^N$ such that $F_i(h_1, x_{1:i-1}, x_i) = u_{2i}$. Hence, for $i \in (i^*+1) : d_2$, $\tilde{x}_i$ is selected recursively as the unique solution of $F_i(h_1^{n^*}, \tilde{x}_{1:i-1}, \tilde{x}_i) = u_{2i}$. This concludes to show that there exists a $\tilde{\mathbf{x}} \in B^N$ such that $\tilde{\mathbf{u}}_2 = F_{K_h}(h_1^{n^*}, \tilde{\mathbf{x}})$ and $\|\mathbf{u}_2 - \tilde{\mathbf{u}}_2\|_\infty \leq C_K C_H r_3(N)^{1/d_1}$. Moreover, since $\tilde{x}_{i^*} = b'_{i^*} = b^N_{i^*}$, we have $\tilde{\mathbf{x}} \in \partial(B^N)$ and therefore $\tilde{\mathbf{u}} \in \partial(E^N(B^N))$.

Finally, note that the set B^N depends only on i^*, the smallest index $i \in 1 : d_2$ such that $u_{2i} \neq F_i(h_1^{n^*-1}, x_{1:i-1}, x_i)$, $\forall \mathbf{x} \in [\boldsymbol{a}', \boldsymbol{b}']$. Defining $D^N_{i^*} = B^N$, this shows that the collection $\{D_i^N\}_{i=1}^{d_2}$ of sets in $\mathcal{B}^N_{[0,1)^{d+1}}$ satisfies the desired properties.

Finally, we may conclude the proof as follows:

$$\|\mathcal{S}(P_h^N) - \pi_h^N \otimes K_h\|_{\mathrm{E}} \leq L^{d_1+d_2} D(\mathbf{u}^{1:N}) + (d_2+1)c_N L^{d_1+d_2-1}\left(D(\mathbf{u}^{1:N}) + L^{-(d_1+d_2)}\right)$$

where the optimal value of L is such that $L = \mathcal{O}\left(D(\mathbf{u}^{1:N})^{-\frac{1}{1+d_1+d_2}}\right)$. Let $r(N) = r_1(N)+2r_2(N)+(2C_KC_H)^{d_1}r_3(N)$. Then, if $r(N)D(\mathbf{u}^{1:N})^{-\frac{d_1}{1+d_1+d_2}} = \mathcal{O}(1)$, L verifies all the conditions above and we have $c_N = \mathcal{O}(1)$. Thus

$$\|\mathcal{S}(P_h^N) - \pi_h^N \otimes K_h\|_{\mathrm{E}} = \mathcal{O}\left(D(\mathbf{u}^{1:N})^{\frac{1}{1+d_1+d_2}}\right).$$

Otherwise, if $r(N)D(\mathbf{u}^{1:N})^{-\frac{d_1}{1+d_1+d_2}} \to +\infty$, let $L = \mathcal{O}(r(N)^{-\frac{1}{d_1}})$. Then $c_N = \mathcal{O}(1)$ and

$$\begin{aligned} L^{d_1+d_2} D(\mathbf{u}^{1:N}) &= \mathcal{O}(r(N))^{\frac{1}{d_1} - \frac{1+d_1+d_2}{d_1}} D(\mathbf{u}^{1:N}) \\ &= \mathcal{O}(r(N)^{1/d_1})\left(\mathcal{O}(r(N))^{-1} D(\mathbf{u}^{1:N})^{\frac{d_1}{1+d_1+d_2}}\right)^{\frac{1+d_1+d_2}{d_1}} \\ &= o\left(r(N)^{1/d_1}\right). \end{aligned}$$

Therefore $\|\mathcal{S}(P_h^N) - \pi_h^N \otimes K_h\|_{\mathrm{E}} = o(1)$, which concludes the proof.

C Consistency: proof of Theorem 1.5

We first prove the following Lemma:

Lemma 1.1. *Let $(\pi^N \otimes K)$ be a sequence of probability measures on $[0,1)^{d_1+d_2}$. Assume that $\|\pi^N - \pi\|_{\mathrm{E}} = o(1)$, $\pi \in \mathcal{P}([0,1)^{d_1})$ and that $F_K(\mathbf{x}_1, \mathbf{x}_2)$ is Hölder continuous with its i-th component strictly increasing in x_{2i}, $i \in 1 : d_2$. Then, as $N \to +\infty$,*

$$\|\pi^N \otimes K - \pi \otimes K\|_{\mathrm{E}} \to 0.$$

To prove this result, let $B_1 \times B_2 \in \mathcal{B}_{[0,1)^{d_1+d_2}}$, $B_2 = [\boldsymbol{a}_2, \boldsymbol{b}_2]$,

$$\begin{aligned} \left|\int_{B_1\times B_2} (\pi^N \otimes K - \pi \otimes K)(\mathrm{d}\mathbf{x}_1, \mathrm{d}\mathbf{x}_2)\right| &= \left|\int_{B_1} K(\mathbf{x}_1, B_2)(\pi^N - \pi)(\mathrm{d}\mathbf{x}_1)\right| \\ &= \left|\int_{B_1} \lambda_{d_2}\left(F_K(\mathbf{x}_1, B_2)\right)(\pi^N - \pi)(\mathrm{d}\mathbf{x}_1)\right|. \end{aligned}$$

The function $\mathbf{x}_1 \to \lambda_{d_2}\left(F_K(\mathbf{x}_1, B_2)\right)$ is continuous and bounded and therefore we proceed as in the proof of Theorem 1.1. But since $\lambda_{d_2}\left(F_K(\mathbf{x}_1, B_2)\right)$ depends on $(\boldsymbol{a}_2, \boldsymbol{b}_2)$ and we want to take the supremum over $\boldsymbol{a}_2, \boldsymbol{b}_2 \in (0,1)^{d_2}$, we need to make

sure that, on a compact set J, for any $\epsilon > 0$ we can find $\eta > 0$ which does not depend on $(\boldsymbol{a}_2, \boldsymbol{b}_2)$ such that, for $\mathbf{x}_1$, $\mathbf{x}'_1 \in J$,

$$\|\mathbf{x}_1 - \mathbf{x}'_1\|_\infty \leq \eta \implies |\lambda_{d_2}(F_K(\mathbf{x}_1, B_2)) - \lambda_{d_2}(F_K(\mathbf{x}'_1, B_2))| \leq \epsilon.$$

To see that this is true, note that $\partial(F_K(\mathbf{x}_1, B_2)) = F_K(\mathbf{x}_1, \partial B_2)$. Hence, for any point $\mathbf{c} \in \partial F_K(\mathbf{x}_1, B_2)$ there exists a $\boldsymbol{p} \in \partial B_2$ such that $\mathbf{c} = F_K(\mathbf{x}_1, \boldsymbol{p})$ and therefore, by the Hölder property of F_K, we have

$$\|\mathbf{x}_1 - \mathbf{x}'_1\|_\infty \leq \eta \implies \|\mathbf{c} - \mathbf{c}'\|_\infty \leq C_K \eta^\kappa, \quad \mathbf{c}' = F_K(\mathbf{x}'_1, \boldsymbol{p}) \in \partial F_K(\mathbf{x}'_1, B_2)$$

where C_K and κ are respectively the Hölder constant and the Hölder exponent of F_K. Let $\tilde{F}_K$ be the continuous extension of F_K on $[0,1]^{d_1+d_2}$ (which exists because F_K is Hölder continuous on $[0,1)^{d_1+d_2}$). Let $w > 0$, $\mathbf{x} \in [0,1)^{d_1}$ and $\boldsymbol{a} \leq \boldsymbol{b}$, $(\boldsymbol{a}, \boldsymbol{b}) \in [0,1]^{2d_2}$. Then, define

$$A^+(w, \mathbf{x}, \boldsymbol{a}, \boldsymbol{b}) = \left\{ \mathbf{u} \in [0,1)^{d_2} : \exists \boldsymbol{p} \in \partial[\boldsymbol{a}, \boldsymbol{b}] \text{ such that } \|\mathbf{u} - \tilde{F}_K(\mathbf{x}, \boldsymbol{p})\|_\infty \leq C_K w^\kappa \right\}$$

and, noting $\tilde{F}_i(\mathbf{x}_1, \mathbf{x}_2)$ the i-th component of $\tilde{F}_K(\mathbf{x}_1, \mathbf{x}_2)$, $i \in 1 : d_2$,

$$A^-(w, \mathbf{x}, \boldsymbol{a}, \boldsymbol{b}) = \Big\{ \mathbf{u} \in \tilde{F}_K(\mathbf{x}, [\boldsymbol{a}, \boldsymbol{b}]) : \ \exists \boldsymbol{p} \in \partial[\boldsymbol{a}, \boldsymbol{b}] \\ \text{such that } |u_i - \tilde{F}_i(\mathbf{x}, \boldsymbol{p})| \geq C_K w^\kappa, \ \forall i \in 1 : d_2 \Big\}.$$

Let $B^* = \{(\boldsymbol{a}, \boldsymbol{b}) \in [0,1]^{2d_2} : a_i \leq b_i \, i \in 1 : d_2\}$ and $f : \mathbb{R}^+ \times [0,1)^{d_1} \times B^* \to [0,1]$ be the mapping

$$(w, \mathbf{x}, \boldsymbol{a}, \boldsymbol{b}) \in \mathbb{R}^+ \times [0,1)^{d_1} \times B^* \mapsto f(w, \mathbf{x}, \boldsymbol{a}, \boldsymbol{b}) = \lambda_{d_2}(A^+(w, \mathbf{x}, \boldsymbol{a}, \boldsymbol{b})) - \lambda_{d_2}(A^-(w, \mathbf{x}, \boldsymbol{a}, \boldsymbol{b})).$$

Note that for a fix w the function $f(w, \cdot)$ is continuous on $[0,1)^d \times B^*$ (as $\tilde{F}_K$ is continuous). Therefore, for all $\mathbf{x}_1$ and $\mathbf{x}'_1$ in J such that $\|\mathbf{x}_1 - \mathbf{x}'_1\| \leq \eta$, we have

$$|\lambda_{d_2}(F_K(\mathbf{x}_1, B_2)) - \lambda_{d_2}(F_K(\mathbf{x}'_1, B_2))| \leq f(\eta, \mathbf{x}_1, \boldsymbol{a}_2, \boldsymbol{b}_2) \leq m(\eta)$$

with

$$m(\eta) := \max_{(\mathbf{x}, \boldsymbol{a}, \boldsymbol{b}) \in J \times B^*} f(\eta, \mathbf{x}, \boldsymbol{a}, \boldsymbol{b}).$$

Because f is continuous and $J \times B^*$ is compact, $m(\eta)$ is continuous so that, for any $\epsilon > 0$, there exists a $\eta > 0$ (that depends only on $m(\cdot)$ and therefore independent of B_2) such that $m(\eta) \leq \epsilon$. This concludes the proof of the Lemma.

We now prove Theorem 1.5. By the result of Hlawka and Mück (1972, "Satz 2") and Assumption 3, $\left(\mathbf{x}_0^{1:N}\right)$ is such that $\|\mathcal{S}(\mathbf{x}_0^{1:N}) - m_0\|_{\mathrm{E}} = o(1)$. In addition, the importance weight function $\mathbb{Q}_0(\mathrm{d}\mathbf{x}_0)/m_0(\mathrm{d}\mathbf{x}_0) = G_0(\mathbf{x}_0)/m_0(G_0)$ is continuous and bounded by Assumption 2. Therefore, $\|\widehat{\mathbb{Q}}_0^N - \mathbb{Q}_0\|_{\mathrm{E}} = o(1)$ by Theorem 1.1.

Assume that the result is true at time $t \geq 0$ and let $P^N_{t+1,h} = (h_t^{1:N}, \mathbf{x}_{t+1}^{1:N})$ where $h_t^n = h(\mathbf{x}_t^{\sigma_t(a_t^n)})$. Then, the result is true at time $t+1$ if

$$\|\mathcal{S}(P^N_{t+1,h}) - \mathbb{Q}_{t,h} \otimes m_{t+1,h}\|_{\mathrm{E}} = o(1). \tag{1.20}$$

To see that, let $G_{t,h}(h_{t-1}, \mathbf{x}_t) = G_t(H(h_{t-1}), \mathbf{x}_t)$ and Ψ_{t+1} be the Bolzmann-Gibbs transformation associated to $G_{t+1,h}$ (see Del Moral, 2004, Definition 2.3.3). Then, the importance weight function

$$\frac{\Psi_{t+1}(\mathbb{Q}_{t,h} \otimes m_{t+1})}{\mathbb{Q}_{t,h} \otimes m_{t+1}}(\mathrm{d}(h_t, \mathbf{x}_{t+1}) = \frac{G_{t+1,h}(h_t, \mathbf{x}_{t+1})}{\mathbb{Q}_t \otimes m_{t+1}(G_{t+1})}$$

is continuous and bounded (by Assumption 2 and the continuity of the Hilbert curve) and therefore Theorem 1.1 implies that $\|\widehat{\mathbb{Q}}^N_{t+1} - \mathbb{Q}_{t+1}\|_{\mathrm{E}} = o(1)$ if (1.20) is verified.

To show (1.20), note that

$$\|\mathcal{S}(P^N_{t+1,h}) - \mathbb{Q}_{t,h} \otimes m_{t+1,h}\|_{\mathrm{E}} \leq \|\mathcal{S}(P^N_{t+1,h}) - \overline{\mathbb{Q}}^N_{t+1,h}\|_{\mathrm{E}} + \|\overline{\mathbb{Q}}^N_{t+1,h} - \mathbb{Q}_{t,h} \otimes m_{t+1,h}\|_{\mathrm{E}}.$$

By the inductive hypothesis, $\|\widehat{\mathbb{Q}}^N_t - \mathbb{Q}_t\|_{\mathrm{E}} = o(1)$ so that, by Theorem 1.3, Assumption 3, the Hölder property of the Hilbert curve and Lemma 1.1,

$$\|\overline{\mathbb{Q}}^N_{t+1,h} - \mathbb{Q}_{t,h} \otimes m_{t+1,h}\|_{\mathrm{E}} = \|\widehat{\mathbb{Q}}^N_{t,h} \otimes m_{t+1,h} - \mathbb{Q}_{t,h} \otimes m_{t+1,h}\|_{\mathrm{E}} = o(1).$$

Finally, note that

$$W_t^n \leq \frac{\|G_t\|_\infty}{\mathcal{S}(P^N_{t,h})(G_{t,h})} = o(1)$$

because $\mathcal{S}(P^N_{t,h})(G_{t,h}) = \mathcal{O}(N^{-1})$ by the inductive hypothesis and the fact that $G_{t,h}$ is continuous and bounded (by Assumption 2 and the continuity of the Hilbert curve). Together with the inductive hypothesis and Assumptions 1, 3-4, this implies that all the assumptions of Theorem 1.4 are verified and therefore $\|\mathcal{S}(P^N_{t+1,h}) - \overline{\mathbb{Q}}^N_{t+1,h}\|_{\mathrm{E}} = o(1)$ as required.

D Stochastic bounds

D.1 Setup of the proof of Theorem 1.6

The result is proved by induction. By Assumption 2 of Theorem 1.5, the weight function $\mathbb{Q}_0(\mathrm{d}\mathbf{x}_0)/m_0(\mathrm{d}\mathbf{x}_0) = G_0(\mathbf{x}_0)/m_0(G_0)$ is continuous and bounded. Therefore, the continuity of $F^{-1}_{m_0}$, the assumptions on $(\mathbf{u}_0^{1:N})$ (Assumptions 1 and 2) and Theorem 1.2 give the result at time $t = 0$.

Assume that the result is true at time $t \geq 0$ and let $\hat{I}_{t+1}^N = \widehat{\mathbb{Q}}_{t+1}^N(\varphi)$ where $\varphi : [0,1)^d \to \mathbb{R}$ verifies the conditions of the theorem. As mentioned previously, iteration $t+1$ of SQMC is a QMC importance sampling step from the proposal distribution $\overline{\mathbb{Q}}_{t+1,h}^N$ to the target $w_{t+1,h}^h(h_t, \mathbf{x}_{t+1})\overline{\mathbb{Q}}_{t+1,h}^N(\mathrm{d}(h_t, \mathbf{x}_{t+1}))$ where

$$w_{t+1,h}^N(h_t, \mathbf{x}_{t+1}) := \frac{G_{t+1,h}(h_t, \mathbf{x}_{t+1})}{C_{t+1}^N}$$

with $C_{t+1}^N = \overline{\mathbb{Q}}_{t+1,h}^N(G_{t+1,h})$ and $G_{t+1,h}$ as in the proof of Theorem 1.5. To bound $\mathrm{Var}\{\hat{I}_{t+1}^N\}$ and $\mathbb{E}|\hat{I}_{t+1} - \mathbb{Q}_{t+1}(\varphi)|$ we therefore naturally want to use expression (1.14) and (1.15) derived in the proof of Theorem 1.2. To that effect, we need to show that, for N large enough and almost surely, the assumptions given in Theorem 1.2 on the weight function and on the point set at hand (Assumption 2 of Theorem 1.2) are satisfied.

To see that the conditions on the weight function are fulfilled, note first that $w_{t+1,h}^N$ is continuous by Assumption 2 of Theorem 1.5 and by the continuity of the Hilbert curve. To show that $w_{t+1,h}^N$ is almost surely bounded for N large enough, first note that, by Assumption 1, it is clear from the proofs of Theorem 1.3 and of Theorem 1.5 that, for all $\epsilon > 0$ and for all $t \geq 0$, there exists a $N_{\epsilon,t}^*$ such that, almost surely,

$$\|\widehat{\mathbb{Q}}_{t,h}^N - \mathbb{Q}_{t,h}\|_{\mathrm{E}} \leq \epsilon, \quad \forall N \geq N_{\epsilon,t}^*.$$

In addition, under the assumptions of the theorem, $(C_{t+1}^N)^{-1}$ is almost surely bounded above and below away from 0, for N large enough. Indeed, by Lemma 1.1 (and using the Hölder property of the Hilbert curve), $\|\overline{\mathbb{Q}}_{t+1,h}^N - \mathbb{Q}_{t,h} \otimes m_{t+1,h}\|_{\mathrm{E}} = o(1)$ and, in particular, under the conditions of the theorem, for any $\delta > 0$, we have, almost surely,

$$\|\overline{\mathbb{Q}}_{t+1,h}^N - \mathbb{Q}_{t,h} \otimes m_{t+1,h}\| \leq \delta \tag{1.21}$$

for N large enough (see the proof of Lemma 1.1 and the proof of Theorem 1.1). Writing $C_{t+1} = \mathbb{Q}_{t,h} \otimes m_{t+1,h}(G_{t+1})$, this observation, together with the fact that

$$|C_{t+1}^N - C_{t+1}| = |\overline{\mathbb{Q}}_{t+1,h}^N(G_{t+1,h}) - \mathbb{Q}_{t,h} \otimes m_{t+1,h}(G_{t+1})|$$

where $G_{t+1,h}$ is continuous and bounded (by Assumption 2 of Theorem 1.5 and the continuity of the Hilbert curve), implies that, almost surely, $C_{t+1} + \delta \geq C_{t+1}^N \geq C_{t+1} - \delta := c_\delta > 0$ for N large enough (computations as in the proof of Theorem 1.1). Hence, almost surely, $\|w_{t+1,h}^N\|_\infty \leq c_\delta^{-1}\|G_{t+1}\|_\infty$, for N large enough.

Finally, to show that the point set $P_{t+1,h}^N$ (defined as in the proof of Theorem 1.5) verifies Assumption 2 of Theorem 1.2, note that, from Theorem 1.5 and under the assumptions of the theorem, for any $\epsilon > 0$ there exists a N_ϵ such that, almost surely, $\|\mathcal{S}(P_{t+1,h}^N) - \mathbb{Q}_{t,h} \otimes m_{t+1,h}\|_{\mathrm{E}} \leq \epsilon$ for all $N \geq N_\epsilon$. Together with (1.21), this shows that, as required, for any $\epsilon > 0$ we have, almost surely and for N large enough, $\|\mathcal{S}(P_{t+1,h}^N) - \overline{\mathbb{Q}}_{t+1,h}^N\|_{\mathrm{E}} \leq \epsilon$.

D.2 Proof of Theorem 1.6: L_2-convergence

Using expression (1.14) given in the proof of Theorem 1.2, we have for N large enough

$$\begin{aligned}\mathrm{Var}\{\hat{I}_{t+1}^N\} \leq \Big[2(1+c_\delta^{-1}\|G_{t+1}\|_\infty)\mathrm{Var}\left\{\mathcal{S}(P_{t+1,h}^N)(w_{t+1,h}^N)\right\}^{1/2} + \\ \left\{1-2\mathbb{E}\left[\mathcal{S}(P_{t+1,h}^N)(\varphi w_{t+1,h}^N)\right]\right\}\mathrm{Var}\left\{\mathcal{S}(P_{t+1,h}^N)(\varphi w_{t+1,h}^N)\right\}^{1/2}\Big]^2.\end{aligned} \tag{1.22}$$

We first bound $\mathrm{Var}\{\mathcal{S}(P_{t+1,h}^N)(w_{t+1,h}^N)\}$. Let $\mathcal{F}_t^N$ be the σ-algebra generated by the point set $(h_{1:t-1}^{1:N}, \mathbf{x}_{1:t}^{1:N})$. Then, by Assumption 2,

$$\mathrm{Var}\left\{\mathcal{S}(P_{t+1,h}^N)(w_{t+1,h}^N)|\mathcal{F}_t^N\right\} \leq C^* r(N)\sigma_N^2$$

with C^* as in the statement of the theorem and $\sigma_N^2 \leq \|w_{t+1,h}^N\|_\infty \leq c_\delta^{-1}\|G_{t+1}\|_\infty$ almost surely and for N large enough. Therefore, since $\mathbb{E}\left[\mathcal{S}(P_{t+1,h}^N)(w_{t+1,h}^N)|\mathcal{F}_t^N\right] = 1$, we have

$$\mathrm{Var}\left\{\mathcal{S}(P_{t+1,h}^N)(w_{t+1,h}^N))\right\} = \mathcal{O}(r(N)). \tag{1.23}$$

Next, we need to bound $\mathrm{Var}\{\mathcal{S}(P_{t+1,h}^N)(\varphi w_{t+1,h}^N)\}$. Note that

$$\overline{\mathbb{Q}}_{t+1}^N\left(\left(C_{t+1}^N\right)^{-2}\varphi^2 G_{t+1}^2\right) \leq \frac{1}{\left(C_{t+1}^N\right)^2}\|G_{t+1}\|_\infty^2\widehat{\mathbb{Q}}_t^N\left(m_{t+1}(\varphi^2)\right),$$

where the last factor is almost surely finite for all N. Indeed, since $\varphi \in L_2(\mathcal{X}, \mathbb{Q}_{t+1})$, $m_{t+1}(\varphi^2)(\mathbf{x}_t)$ is finite for almost all $\mathbf{x}_t \in \mathcal{X}$ and the integral with respect to $\widehat{\mathbb{Q}}_t^N$ is a finite sum. Hence, for all N, $\varphi \in L_2(\mathcal{X}^2, \overline{\mathbb{Q}}_{t+1,h}^N)$ almost surely so that, by Assumption 2, we have almost surely

$$\mathrm{Var}\left\{\mathcal{S}(P_{t+1,h}^N)(\varphi w_{t+1,h}^N)|\mathcal{F}_t^N\right\} \leq C^* r(N)\sigma_{N,\varphi}^2$$

where, with probability one and for N large enough, $\sigma_{N,\varphi}^2 \leq c_\delta^{-2}\|G_{t+1}\|_\infty^2\overline{\mathbb{Q}}_{t+1}^N(\varphi^2)$. We now need to show that $\mathbb{E}[\overline{\mathbb{Q}}_{t+1}^N(\varphi^2)]$ is bounded.

In order to establish this, we prove that for all $t \geq 0$ and for N large enough, we have, $\forall f \in L_1(\mathcal{X}^2, \mathbb{Q}_t \otimes m_{t+1})$,

$$\mathbb{E}[\overline{\mathbb{Q}}_{t+1}^N(f)] \leq c_{t+1}\mathbb{Q}_t \otimes m_{t+1}(|f|) \tag{1.24}$$

for constant c_{t+1}.

Equation (1.24) is true for $t = 0$. Indeed, let $f \in L_1(\mathcal{X}^2, \mathbb{Q}_0 \otimes m_1)$ and note that, under the conditions of the theorem, almost surely and for N large enough, $\{\mathcal{S}(\mathbf{x}_0^{1:N})(G_0)\}^{-1} \leq \tilde{c}_0 < \infty$ for a constant $\tilde{c}_0$. Hence, for N large enough, we have

$$\begin{aligned}\mathbb{E}[\overline{\mathbb{Q}}_1^N(f)] &= \mathbb{E}\left[\left\{\mathcal{S}(\mathbf{x}_0^n)(G_0)\right\}^{-1}\frac{1}{N}\sum_{n=1}^N G_0(\mathbf{x}_0^n)\int_{\mathcal{X}} f(\mathbf{x}_0^n, \mathbf{x}_1)m_1(\mathbf{x}_0^n, \mathrm{d}\mathbf{x}_1)\right] \\ &\leq c_0\mathbb{Q}_0 \otimes m_1(|f|)\end{aligned}$$

with $c_0 = \tilde{c}_0 m_0(G_0)$. Assume that (1.24) is true for $t \geq 0$ and note that, under the conditions of the theorem, almost surely and for N large enough, $\{\mathcal{S}(P_t^N)(G_t)\}^{-1} \leq \tilde{c}_t < \infty$ for a constant $\tilde{c}_t$. Then, for N large enough (with the convention $G_t(\mathbf{x}_{t-1}, \mathbf{x}_t) = G_0(\mathbf{x}_0)$ if $t = 0$),

$$\begin{aligned}
\mathbb{E}[\overline{\mathbb{Q}}_{t+1}^N(f)] &= \mathbb{E}\left[\left\{\mathcal{S}(P_t^N)(G_t)\right\}^{-1} \frac{1}{N}\sum_{n=1}^N G_t(\mathbf{x}_{t-1}^{\sigma_{t-1}(a_{t-1}^n)}, \mathbf{x}_t^n) \int_{\mathcal{X}} f(\mathbf{x}_t^n, \mathbf{x}_{t+1}) m_{t+1}(\mathbf{x}_t^n, \mathrm{d}\mathbf{x}_{t+1})\right] \\
&\leq \tilde{c}_t \frac{1}{N}\sum_{n=1}^N \mathbb{E}\left\{\mathbb{E}\left[\int_{\mathcal{X}} G_t(\mathbf{x}_{t-1}^{\sigma_{t-1}(a_{t-1}^n)}, \mathbf{x}_t^n)|f(\mathbf{x}_t^n, \mathbf{x}_{t+1})| m_{t+1}(\mathbf{x}_t^n, \mathrm{d}\mathbf{x}_{t+1})|\mathcal{F}_t^N\right]\right\} \\
&= \tilde{c}_t \mathbb{E}\left[\int_{\mathcal{X}^3} G_t(\mathbf{x}_{t-1}, \mathbf{x}_t)|f(\mathbf{x}_t, \mathbf{x}_{t+1})| \overline{\mathbb{Q}}_t^N \otimes m_{t+1}(\mathrm{d}\mathbf{x}_{t-1:t+1})\right] \\
&\leq \tilde{c}_t c_{t-1} \int_{\mathcal{X}^3} G_t(\mathbf{x}_{t-1}, \mathbf{x}_t)|f(\mathbf{x}_t, \mathbf{x}_{t+1})| \mathbb{Q}_{t-1} \otimes m_t \otimes m_{t+1}(\mathrm{d}\mathbf{x}_{t-1:t+1}) \\
&= c_t \int_{\mathcal{X}^3} |f(\mathbf{x}_t, \mathbf{x}_{t+1})| \Psi_t\left(\mathbb{Q}_{t-1} \otimes m_t\right) \otimes m_{t+1}(\mathrm{d}\mathbf{x}_{t-1:t+1})) \\
&= c_t \int_{\mathcal{X}^2} |f(\mathbf{x}_t, \mathbf{x}_{t+1})| \mathbb{Q}_t \otimes m_{t+1}(\mathrm{d}\mathbf{x}_{t:t+1}) \\
&= c_t \mathbb{Q}_t \otimes m_{t+1}(|f|)
\end{aligned}$$

with $c_t = c_{t-1}\tilde{c}_t\left[\mathbb{Q}_{t-1} \otimes m_t(G_t)\right]$, Ψ_t be the Bolzmann-Gibbs transformation associated to G_t (see Del Moral, 2004, Definition 2.3.4) and where the second inequality uses the inductive hypothesis and the fact that the mapping

$$(\mathbf{x}_{t-1}, \mathbf{x}_t) \mapsto G_t(\mathbf{x}_{t-1}, \mathbf{x}_t) m_{t+1}(|f|)(\mathbf{x}_t)$$

belongs to $L_1(\mathcal{X}^2, \mathbb{Q}_{t-1} \otimes m_t)$. This shows (1.24) and therefore, for N large enough, $\mathbb{E}[\sigma_{N,\varphi}^2] \leq c$ for a constant c so that $\mathbb{E}[\mathrm{Var}\{\mathcal{S}(P_{t+1,h}^N)(\varphi w_{t+1,h}^N)\big|\mathcal{F}_t^N\}] = \mathcal{O}(r(N))$. In addition

$$\begin{aligned}
\mathbb{E}\left[\mathcal{S}(P_{t+1,h}^N)(\varphi w_{t+1,h}^N)|\mathcal{F}_t^N\right] &= \frac{\widehat{\mathbb{Q}}_t^N\left(m_{t+1}(\varphi G_{t+1})\right)}{C_{t+1}^N} \\
&= \frac{\mathbb{Q}_t\left(m_{t+1}(\varphi G_{t+1})\right)}{C_{t+1}^N} + \frac{(\widehat{\mathbb{Q}}_t^N - \mathbb{Q}_t)\left(m_{t+1}(\varphi G_{t+1})\right)}{C_{t+1}^N}
\end{aligned}$$

where $\mathbb{Q}_t\left(m_{t+1}(\varphi G_{t+1})\right) < +\infty$ because $\varphi \in L_2(\mathcal{X}, \mathbb{Q}_{t+1})$. Since

$$\frac{\mathbb{Q}_t\left(m_{t+1}(\varphi G_{t+1})\right)}{C_{t+1}^N} = C_{t+1}^{-1}\mathbb{Q}_t\left(m_{t+1}(\varphi G_{t+1})\right) + \frac{C_{t+1} - C_{t+1}^N}{C_{t+1}^N C_{t+1}}\mathbb{Q}_t\left(m_{t+1}(\varphi G_{t+1})\right),$$

we therefore have, for N large enough,

$$\mathrm{Var}\left\{\frac{\mathbb{Q}_t\left(m_{t+1}(\varphi G_{t+1})\right)}{C_{t+1}^N}\right\} = \left[\mathbb{Q}_t\left(m_{t+1}(\varphi G_{t+1})\right)\right]^2 \mathrm{Var}\left\{\frac{C_{t+1}-C_{t+1}^N}{C_{t+1}^N C_{t+1}}\right\}$$
$$\leq \frac{\left[\mathbb{Q}_t\left(m_{t+1}(\varphi G_{t+1})\right)\right]^2}{(c_\delta C_{t+1})^2}\mathbb{E}\left[\left\{\left(\widehat{\mathbb{Q}}_t^N - \mathbb{Q}_t\right)\left(m_{t+1}(G_{t+1})\right)\right\}^2\right].$$

Since $\|G_{t+1}\|_\infty < +\infty$, $m_{t+1}(G_{t+1})$ is bounded and the inductive hypothesis implies that the term on the right of the inequality sign is $\mathcal{O}(r(N))$. In addition, for all N large enough,

$$\mathrm{Var}\left\{\frac{1}{C_{t+1}^N}\left(\widehat{\mathbb{Q}}_t^N - \mathbb{Q}_t\right)\left(m_{t+1}(\varphi G_{t+1})\right)\right\} \leq c_\delta^{-2}\mathbb{E}\left[\left\{\left(\widehat{\mathbb{Q}}_t^N - \mathbb{Q}_t\right)\left(m_{t+1}(\varphi G_{t+1})\right)\right\}^2\right].$$

Since $\left[m_{t+1}(\varphi G_{t+1})(\mathbf{x}_t)\right]^2 \leq \|G_{t+1}\|_\infty m_{t+1}(\varphi^2 G_{t+1})(\mathbf{x}_t)$, we have

$$\mathbb{Q}_t(\{m_{t+1}(\varphi G_{t+1})\}^2) \leq \|G_{t+1}\|_\infty C_{t+1}\mathbb{Q}_{t+1}(\varphi^2) < +\infty$$

by assumption. Therefore, $m_{t+1}(\varphi G_{t+1}) \in L_2(\mathcal{X}, \mathbb{Q}_t)$ so that, by the inductive hypothesis, $\mathrm{Var}\{\mathbb{E}[\mathcal{S}(P_{t+1,h}^N)(\varphi w_{t+1,h}^N)|\mathcal{F}_t^N]\} = \mathcal{O}(r(N))$. Hence,

$$\mathrm{Var}\left\{\mathcal{S}(P_{t+1,h}^N)(\varphi w_{t+1,h}^N)\right\} = \mathcal{O}(r(N)). \tag{1.25}$$

The last term of (1.22) we need to control is

$$\mathbb{E}\left[\mathcal{S}(P_{t+1,h}^N)(\varphi w_{t+1,h}^N)\right] = \mathbb{E}\left[\frac{1}{C_{t+1}^N}\widehat{\mathbb{Q}}_t^N(m_{t+1}(\varphi G_{t+1}))\right].$$

Since we saw that $m_{t+1}(\varphi G_{t+1}) \in L_2(\mathcal{X}, \mathbb{Q}_t)$, we have, for N large enough,

$$\begin{aligned}\mathbb{E}\left[\mathcal{S}(P_{t+1,h}^N)(\varphi w_{t+1,h}^N)\right] &= \mathbb{E}\left[\frac{1}{C_{t+1}^N}\right]\mathbb{Q}_t(m_{t+1}(\varphi G_{t+1})) \\ &\quad + \mathbb{E}\left[\frac{1}{C_{t+1}^N}(\widehat{\mathbb{Q}}_t^N - \mathbb{Q}_t)(m_{t+1}(\varphi G_{t+1}))\right] \\ &\leq c_\delta^{-1}\left[\mathbb{Q}_t(m_{t+1}(\varphi G_{t+1})) + \mathcal{O}(r(N)^{1/2})\right]\end{aligned} \tag{1.26}$$

using previous computations.

Combining (1.22), (1.23), (1.25) and (1.26), one obtains $\mathrm{Var}\{\hat{I}_{t+1}^N\} = \mathcal{O}(r(N))$.

D.3 Proof of Theorem 1.6: L_1-convergence

Let $I_{t+1} = \mathbb{Q}_{t+1}(\varphi)$ and $I_{t+1}^N = \mathbb{Q}_{t+1}^N(\varphi)$ so that

$$\mathbb{E}[|\hat{I}_{t+1}^N - I_{t+1}|] \leq \mathbb{E}[|\hat{I}_{t+1}^N - I_{t+1}^N|] + \mathbb{E}[|I_{t+1}^N - I_{t+1}|].$$

Then, using expression (1.15) in the proof of Theorem 1.2, we have, for N large enough,

$$\begin{aligned}\mathbb{E}\left[|\hat{I}_{t+1}^N - I_{t+1}^N|\right] &\leq \mathrm{Var}\left\{\mathcal{S}(P_{t+1,h}^N)(\varphi w_{t+1,h}^N)\right\}^{1/2} + 2\left(\mathrm{Var}\left\{\mathcal{S}(P_{t+1,h}^N)(\varphi w_{t+1,h}^N)\right\}\right. \\ &\quad \left. + \left\{\mathbb{E}\left[\mathcal{S}(P_{t+1,N})(\varphi w_{t+1,h}^N)\right]\right\}^2\right)^{1/2} \mathrm{Var}\left\{\mathcal{S}(P_{t+1,h}^N)(w_{t+1,h}^N)\right\}^{1/2} \\ &= \mathcal{O}(r(N)^{1/2})\end{aligned}$$

from above computations. In addition,

$$\begin{aligned}\mathbb{E}\left[|I_{t+1}^N - I_{t+1}|\right] &= \mathbb{E}\left[\left|\left(\frac{\widehat{\mathbb{Q}}_t^N}{C_{t+1}^N} - \frac{\mathbb{Q}_t}{C_{t+1}}\right)(m_{t+1}(\varphi G_{t+1}))\right|\right] \\ &\leq \mathbb{E}\left[\frac{1}{C_{t+1}}\left|(\widehat{\mathbb{Q}}_t^N - \mathbb{Q}_t)(m_{t+1}(\varphi G_{t+1}))\right|\right] \\ &\quad + \mathbb{E}\left|\frac{|C_{t+1} - C_{t+1}^N|}{C_{t+1}^N C_{t+1}}\widehat{\mathbb{Q}}_t^N(m_{t+1}(\varphi G_{t+1}))\right|.\end{aligned}$$

By the inductive hypothesis and the above computations, the first term after the inequality sign is $\mathcal{O}(r(N)^{1/2})$. In addition, for N large enough, the second term after the inequality sign is bounded by

$$\begin{aligned}\mathbb{E}\left|\frac{|C_{t+1} - C_{t+1}^N|}{C_{t+1}^N C_{t+1}}\widehat{\mathbb{Q}}_t^N(m_{t+1}(\varphi G_{t+1}))\right| &\leq \frac{\delta}{c_\delta C_{t+1}}\mathbb{E}\left|(\widehat{\mathbb{Q}}_t^N - \mathbb{Q}_t)(m_{t+1}(\varphi G_{t+1}))\right| \\ &\quad + \frac{|\mathbb{Q}_t(m_{t+1}(\varphi G_{t+1})|}{c_\delta C_{t+1}}\mathbb{E}\left|(\widehat{\mathbb{Q}}_t^N - \mathbb{Q}_t)(m_{t+1}(G_{t+1}))\right|.\end{aligned}$$

We saw above that the first term on the right-hand side is $\mathcal{O}(r(N)^{1/2})$. In addition, $m_{t+1}(G_{t+1})$ belongs to $L_2(\mathcal{X}, \mathbb{Q}_t)$ because $\|G_{t+1}\|_\infty < +\infty$. Hence, by the inductive hypothesis, the second term after the inequality sign is also $\mathcal{O}(r(N)^{1/2})$ and the proof is complete.

D.4 Proof of Theorem 1.7

To avoid confusion between the t of the time index and the t of the (t, s)-sequence we replace the latter by $\tilde{t}$ in what follows.

The result is true at time $t = 0$ by Theorem 1.2. To obtain the result for $t \geq 1$ we need to modify the steps in the proof of Theorem 1.6 where we do not use the inductive hypothesis. Inspection of this proof shows that we only need to establish that, for any function $\varphi \in \mathcal{C}_b([0,1)^{1+d})$, we have

$$\mathbb{E}\left[\mathrm{Var}\left(\mathcal{S}(P_{t+1,h}^N)(\varphi)|\mathcal{F}_t^N\right)\right] = o(N^{-1}).$$

Let $N = \lambda b^m$. Then, from the proof of Owen (1998, Theorem 1), and using the same notations as in that paper (note in particular the new meaning for symbol u), we have

$$\mathrm{Var}\left(\mathcal{S}(P^N_{t+1,h})(\varphi)|\mathcal{F}^N_t\right) \leq \frac{c}{N}\sum_{|u|>0}\sum_{|\kappa|>m-\tilde{t}-|u|}\sigma^2_{N,u,\kappa}$$

for a constant c, where $|u|$ is the cardinal of $u \subseteq \{1,...,d+1\}$, κ is a vector of $|u|$ nonnegative integers k_j, $j \in u$, and $|\kappa| = \sum_{j\in u} k_j$. Note that κ depends implicitly on u. The $\sigma^2_{N,u,\kappa}$'s are such that

$$\sigma^2_N = \overline{\mathbb{Q}}^N_{t+1,h}(\varphi^2) - \overline{\mathbb{Q}}^N_{t+1,h}(\varphi)^2 = \sum_{|u|>0}\sum_{\kappa}\sigma^2_{N,u,\kappa},$$

with $\sigma^2_{N,u,\kappa} = \int_{[0,1)^{1+d}} \nu_{N,u,\kappa}(\mathbf{x})^2 \mathrm{d}\mathbf{x}$ and

$$\nu_{N,u,\kappa}(\mathbf{x}) = \sum_{\tau(u,\kappa)}\sum_{\gamma(u)} < \varphi \circ F^{-1}_{\overline{\mathbb{Q}}^N_{t+1,h}}, \psi_{u,\kappa,\tau,\gamma} > \psi_{u,\kappa,\tau,\gamma}(\mathbf{x})$$

where $< f_1, f_2 >= \int f_1(\mathbf{x}) f_2(\mathbf{x}) \mathrm{d}\mathbf{x}$, $\psi_{u,\kappa,\tau,\gamma}$ is bounded and all the sums in the definition of $\nu_{N,u,\kappa}(\mathbf{x})$ are finite (see Owen, 1997a, for more details).

Similarly, let

$$\sigma^2 = \mathbb{Q}_{t,h} \otimes m_{t+1,h}(\varphi^2) - \mathbb{Q}_{t,h} \otimes m_{t+1,h}(\varphi)^2 = \sum_{|u|>0}\sum_{\kappa}\sigma^2_{u,\kappa},$$

where $\sigma^2_{u,\kappa} = \int_{[0,1)^{1+d}} \nu_{u,\kappa}(\mathbf{x})^2 \mathrm{d}\mathbf{x}$ and with

$$\nu_{u,\kappa}(\mathbf{x}) = \sum_{\tau(u,\kappa)}\sum_{\gamma(u)} < \varphi \circ F^{-1}_{\mathbb{Q}_{t,h}\otimes m_{t+1,h}}, \psi_{u,\kappa,\tau,\gamma} > \psi_{u,\kappa,\tau,\gamma}(\mathbf{x}).$$

We first want to establish that $|\sigma^2_{N,u,\kappa} - \sigma^2_{u,\kappa}| = o(1)$ almost surely. Note that

$$\|\nu_{N,u,\kappa} - \nu_{u,\kappa}\|_\infty \leq c \sum_{\tau(u,\kappa)}\sum_{\gamma(u)} \left| < \varphi \circ F^{-1}_{\overline{\mathbb{Q}}^N_{t+1,h}}, \psi_{u,\kappa,\tau,\gamma} > - < \varphi \circ F^{-1}_{\mathbb{Q}_{t,h}\otimes m_{t+1,h}}, \psi_{u,\kappa,\tau,\gamma} > \right|$$

for a constant $c > 0$. To show that the term inside the absolute value sign is almost surely $o(1)$, assume that for all $\tilde{u} \in [0,1)$, $|F^{-1}_{\widehat{\mathbb{Q}}^N_{t,h}}(\tilde{u}) - F^{-1}_{\mathbb{Q}_{t,h}}(\tilde{u})| = o(1)$ almost surely. Using the continuity of φ and the continuity of the Hilbert curve H, and the fact that that $F^{-1}_{m_{t+1}}(\mathbf{x}_t, \mathbf{x}_{t+1})$ is a continuous function of $\mathbf{x}_t$ (Assumption 2), we have for any $(h_t, \mathbf{x}_{t+1}) \in [0,1)^{d+1}$

$$\left|\varphi \circ F^{-1}_{\overline{\mathbb{Q}}^N_{t+1,h}}(h_t, \mathbf{x}_{t+1}) - \varphi \circ F^{-1}_{\mathbb{Q}_{t,h}\otimes m_{t+1,h}}(h_t, \mathbf{x}_{t+1})\right| = o(1), \quad \text{a.s.}$$

and therefore, since φ and $\psi_{u,\kappa,\tau,\gamma}$ are bounded, we have, by the dominated convergence Theorem,

$$\left| < \varphi \circ F^{-1}_{\overline{\mathbb{Q}}^N_{t+1,h}}, \psi_{u,\kappa,\tau,\gamma} > - < \varphi \circ F^{-1}_{\mathbb{Q}_{t,h} \otimes m_{t+1,h}}, \psi_{u,\kappa,\tau,\gamma} > \right| \to 0, \quad \text{a.s.}$$

We now establish that, for all $\tilde{u} \in [0,1)$, $|F^{-1}_{\widehat{\mathbb{Q}}^N_{t,h}}(\tilde{u}) - F^{-1}_{\mathbb{Q}_{t,h}}(\tilde{u})| \to 0$ almost surely. The proof of this result is inspired from Barvínek et al. (1991, Theorem 2).

First, note that because $p_t(\mathbf{x}_t) > 0$ for all $\mathbf{x}_t \in [0,1)^d$ (Assumption 4 of Theorem 1.5) the function $F_{\mathbb{Q}_{t,h}}$ is continuous and strictly increasing on $[0,1)$ (see the proof of Lemma 1.1). Let $\epsilon > 0$ and $\tilde{u}_1 \in [0,1)$. Then, by the continuity of $F^{-1}_{\mathbb{Q}_{t,h}}$, there exists a $\delta_{\tilde{u}_1,\epsilon} > 0$ such that,

$$|\tilde{u}_1 - \tilde{u}| \leq \delta_{\tilde{u}_1,\epsilon}, \quad \Longrightarrow \; |F^{-1}_{\mathbb{Q}_{t,h}}(\tilde{u}_1) - F^{-1}_{\mathbb{Q}_{t,h}}(\tilde{u})| \leq \epsilon. \tag{1.27}$$

In the proof of Theorem 1.6 we saw that, for any $\delta_0 > 0$, there exists a N_{δ_0} such that, for all $N \geq N_{\delta_0}$,

$$\|F_{\widehat{\mathbb{Q}}^N_{t,h}} - F_{\mathbb{Q}_{t,h}}\|_\infty \leq \delta_0, \quad \text{a.s.} \tag{1.28}$$

Let $x_N = F^{-1}_{\widehat{\mathbb{Q}}^N_{t,h}}(\tilde{u}_1)$ and $u_N = F_{\mathbb{Q}_{t,h}}(x_N)$. Then, by (1.28),

$$|F_{\widehat{\mathbb{Q}}^N_{t,h}}(x_N) - F_{\mathbb{Q}_{t,h}}(x_N)| \leq \delta_0, \quad \forall N \geq N_{\delta_0}, \quad \text{a.s.}$$

Let $r_N(\tilde{u}_1) = F_{\widehat{\mathbb{Q}}^N_{t,h}}(F^{-1}_{\widehat{\mathbb{Q}}^N_{t,h}}(\tilde{u}_1)) - \tilde{u}_1$ so that

$$|F_{\widehat{\mathbb{Q}}^N_{t,h}}(x_N) - F_{\mathbb{Q}_{t,h}}(x_N)| = |\tilde{u}_1 + r_N(\tilde{u}_1) - u_N| \leq \delta_0, \quad \forall N \geq N_{\delta_0}, \quad \text{a.s.}$$

Now note that $|r_N(\tilde{u}_1)| \leq \frac{\|G_t\|_\infty}{N\mathcal{S}(P_t^N)(G_t)}$ a.s.. Then, it is easy to see that, for all $\delta' > 0$, there exists a $N_{\delta'}$ such that, a.s., $|r_N(\tilde{u}_1)| \leq \delta'$ for all $N \geq N_{\delta'}$. Let $\delta = \delta_0 + \delta'$ and set $N_\delta := N_{\delta_0} \vee N_{\delta'}$. Then, for $N \geq N_\delta$, we have almost surely $|\tilde{u}_1 - u_N| \leq \delta$. By taking δ_0 and δ' such that $\delta = \delta_{\tilde{u}_1,\epsilon}$, (1.27) implies that

$$|F^{-1}_{\mathbb{Q}_{t,h}}(\tilde{u}_1) - F^{-1}_{\mathbb{Q}_{t,h}}(u_N)| \leq \epsilon, \quad \forall N \geq N_{\delta_{\tilde{u}_1,\epsilon}}, \quad \text{a.s.}$$

In addition, $F^{-1}_{\mathbb{Q}_{t,h}}(u_N) = x_N = F^{-1}_{\widehat{\mathbb{Q}}^N_{t,h}}(\tilde{u}_1)$ and therefore , $\forall N \geq N_{\delta_{\tilde{u}_1},\epsilon}$,

$$|F^{-1}_{\mathbb{Q}_{t,h}}(\tilde{u}_1) - F^{-1}_{\widehat{\mathbb{Q}}^N_{t,h}}(\tilde{u}_1)| \leq \epsilon, \quad \text{a.s.}$$

Consequently, $\|\nu_{N,u,\kappa} - \nu_{u,\kappa}\|_\infty = o(1)$ almost surely so that, by the dominated convergence Theorem, $\sigma^2_{N,u,\kappa} \to \sigma^2_{u,\kappa}$ almost surely. Also, because φ is continuous and bounded, $\sigma^2_N \to \sigma^2$ almost surely by Theorem 1.5 and portmanteau lemma (Van der Vaart, 2007, Lemma 2.2). To simplify the notations in what follows, let

$\tilde{\sigma}^2_{u,l} = \sum_{\kappa:|\kappa|=l} \sigma^2_{u,\kappa}$ and $\tilde{\sigma}^2_{N,u,l} = \sum_{\kappa:|\kappa|=l} \sigma^2_{N,u,\kappa}$ (remark that l depends implicitly on u), and note that, for $m \geq \tilde{t} + d + 1$,

$$\sum_{|u|>0} \sum_{l>m-\tilde{t}-|u|} \tilde{\sigma}^2_{N,u,l} = \sigma^2_N - \sum_{|u|>0} \sum_{l=0}^{\infty} \mathbb{I}(l \leq m - \tilde{t} - |u|) \tilde{\sigma}^2_{N,u,\kappa}.$$

By Fubini's Theorem,

$$\mathbb{E}\left[\sum_{|u|>0} \sum_{l>m-\tilde{t}-|u|} \tilde{\sigma}^2_{N,u,l}\right] = \mathbb{E}[\sigma^2_N] - \sum_{|u|>0} \sum_{l=0}^{\infty} \mathbb{I}(l \leq m - \tilde{t} - |u|) \mathbb{E}[\tilde{\sigma}^2_{N,u,l}]$$

where, by the dominated convergence Theorem, $\mathbb{E}[\sigma^2_N] \to \sigma^2$. In addition, since in the definition of $\tilde{\sigma}^2_{N,u,l}$ and $\tilde{\sigma}^2_{u,l}$ the notation $\sum_{\kappa:|\kappa|=l}$ denotes a finite sum, we have, for any u and l, $\tilde{\sigma}^2_{N,u,l} \to \tilde{\sigma}^2_{u,l}$ almost surely and therefore, by the dominated convergence Theorem, $\mathbb{E}[\tilde{\sigma}^2_{N,u,\kappa}] \to \tilde{\sigma}^2_{u,\kappa}$ (because $\tilde{\sigma}^2_N$ is bounded by $\|\varphi\|^2_\infty$). Hence, using Fatou's lemma,

$$\begin{aligned}
0 &\leq \limsup_{m\to+\infty} \mathbb{E}\left[\sigma^2_N - \sum_{|u|>0} \sum_{l=0}^{\infty} \mathbb{I}(l \leq m - \tilde{t} - |u|) \tilde{\sigma}^2_{N,u,l}\right] \\
&\leq \limsup_{m\to+\infty} \mathbb{E}[\sigma^2_N] + \limsup_{m\to+\infty} \left\{ - \sum_{|u|>0} \sum_{l=0}^{\infty} \mathbb{I}(l \leq m - \tilde{t} - |u|) \mathbb{E}[\tilde{\sigma}^2_{N,u,l}] \right\} \\
&\leq \sigma^2 - \sum_{|u|>0} \sum_{l=0}^{\infty} \liminf_{m\to+\infty} \mathbb{I}(l \leq m - \tilde{t} - |u|) \mathbb{E}[\tilde{\sigma}^2_{N,u,l}] \\
&= \sigma^2 - \sum_{|u|>0} \sum_{l=0}^{\infty} \tilde{\sigma}^2_{u,l} = 0,
\end{aligned}$$

since the indicator functions converge to one.

Chapter 2

Convergence Results for Quasi-Monte Carlo Smoothing Algorithms

Joint work with Nicolas Chopin (ENSAE/CREST)

Abstract

Sequential quasi-Monte Carlo (SQMC) algorithms were recently introduced by Gerber and Chopin (2014) as an efficient way to solve filtering problems in state-space models. In Gerber and Chopin (2014) a backward step for SQMC is suggested and a numerical study shows that the resulting quasi-Monte Carlo (QMC) forward-backward smoothing algorithm outperforms its Monte Carlo counterpart. However, no theoretical justification concerning the validity of this method is provided. In this work we contribute to fill this gap by proposing asymptotic results. We also show how the present analysis can be used to study a QMC version of other smoothing strategies such as two filter smoothing (Briers et al., 2010). As a preliminary step for our analysis, we provide a general result on the conversion of discrepancies through the Hilbert space filling curve as well as a generalization of the classical result of Hlawka and Mück (1972) on the transformation of QMC point sets into low discrepancy point sets with respect to non uniform distributions. As a corollary of this latter, we note that we can slightly weaken the assumptions to prove the consistency of SQMC.

Keywords: Low discrepancy; Particle filtering; Quasi-Monte Carlo; Sequential quasi-Monte Carlo; Smoothing;

2.1 Introduction

State-space models are popular tools to model real life phenomena in many fields such as Economics, Engineering and Neuroscience. These models are mainly used for extracting information about a hidden Markov process $(\mathbf{x}_t)_{t\geq 0}$ of interest from a set of $T+1$ observations $\mathbf{y}_{0:T} := (\mathbf{y}_0, \ldots, \mathbf{y}_T)$. In practice, this typically translates to the estimation of $p(\mathbf{x}_t|\mathbf{y}_{0:t})$, the distribution of $\mathbf{x}_t$ given the data $\mathbf{y}_{0:t}$, (called the *filtering* distribution) and/or to $p(\mathbf{x}_{0:T}|\mathbf{y}_{0:T})$ (called the *smoothing* distribution). Nevertheless, except in very specific scenarios, it is well known that both of these distributions are intractable and therefore approximation techniques have to be used, such as extended Kalman filter methods or particle filtering.

Recently, Gerber and Chopin (2014) have introduced sequential quasi-Monte Carlo (SQMC) algorithms as an efficient tool to carry out statistical inference in state-space models. SQMC is a quasi-Monte Carlo version of standard particle filtering algorithms (see e.g. Doucet et al., 2001) where all the underlying uniform pseudo-random numbers are replaced by QMC point sets. Informally, a QMC point set is a deterministic set of points that looks "more uniform" than a random sample of uniform variates. A randomized version of SQMC is obtained by using randomized QMC (RQMC) point sets which combine the advantage of random sampling and QMC strategies, namely to both spread evenly over unit hypercubes and to be such that marginally every point is uniformly distributed. Based on results on RQMC quadrature rules, Gerber and Chopin (2014) establish that for some constructions of RQMC point sets the worst case convergence rate of the randomized SQMC algorithm is at least as fast as for Monte Carlo filtering algorithms, while SQMC outperforms Monte Carlo filtering methods with an error of size $o_P(N^{-1/2})$ on the class of continuous and bounded functions, where N is the number of simulations (or "particles").

Concerning the estimation of the smoothing distribution, Gerber and Chopin (2014) evoke an intuitive way to extend SQMC to carry out forward the estimation of this distribution. Nevertheless, forward algorithms yield very imprecise approximations due to the well known weight degeneracy problems (see Doucet et al., 2000, for a discussion). To overcome this issue, more efficient methods have been proposed in the literature, the first and the most popular of them being the forward-backward smoothing algorithm (Doucet et al., 2000; Godsill et al., 2004). A QMC backward step for SQMC is proposed in Gerber and Chopin (2014) and it is shown in a numerical study that, for a given number of particles, this QMC forward-backward smoothing algorithm leads to important gain compared to its Monte Carlo counterpart. Since the complexity of backward smoothing is $\mathcal{O}(N^2)$, these gains obtained for a fix number of particles translate into impressing savings in term of running time. However, as for QMC forward smoothing, no consistency results for this algorithm is provided.

The main objective of this work is to fill these gaps. We first briefly show that

QMC forward smoothing indeed yields a consistent approximation of the distribution of interest. Then, we establish that the SQMC estimates of the filtering distributions can be merged together, through the backward decomposition of the smoothing distribution (Del Moral et al., 2010), to get a consistent approximation of $p(\mathbf{x}_{0:T}|\mathbf{y}_{0:T})$. Next, we prove the L_2-convergence of QMC forward-backward smoothing for continuous and bounded test functions before providing a consistency result. To establish the consistency of SQMC (Gerber and Chopin, 2014, Theorem 5), the main technical difficulty is to deal with the discontinuities of the algorithm. In this work, we choose a simpler approach than the one used in Gerber and Chopin (2014). In a first step, we study a continuous version of the backward step while, in a second step, we provide simple conditions to show how results obtained for this latter can serve to provide sufficient conditions for the validity of QMC forward-backward smoothing. Although these conditions are rather strong, the advantage of this approach is that it prevents us to be distracted by complicated discontinuity issues for which we refer to Gerber and Chopin (2014, Theorem 4) for a more elegant solution. We also propose and establish the validity of a QMC backward step designed to estimated the marginal smoothing distributions, that is, the law of $\mathbf{x}_t$ given the complete set of observation $\mathbf{y}_{0:T}$. Compared to the forward-backward method which aims to estimate the full smoothing distribution, this algorithm has the advantage to rely on QMC point sets of dimension 1 and is therefore much more efficient to estimate the marginal distributions. Finally, we explain how our analysis may serve to establish the validity of QMC version of other smoothing strategies such as, for instance, two filter smoothing (Briers et al., 2010).

As preliminary computations we propose two results on low discrepancy point sets with respect to non uniform distributions. The first one is a generalization of the classical result of Hlawka and Mück (1972) on the transformation of QMC point sets into low discrepancy point sets with respect to non uniform distributions, while the second one is a general result about discrepancy conversions through the Hilbert space filling curve. When applied on discrepancies with respect to the uniform distribution, this latter extends the result of He and Owen (2014, Theorem 3.2) obtained for the van der Corput sequence to any construction of QMC point sets (although, when applied to the first N points of the van der Corput sequence, the rate we obtain for the discrepancy has an extra $(\log N)^{1/d}$ term, with d the dimension of the resulting point set).

The rest of this paper is organized as follows. Section 2.2 presents the background material we need to study the backward pass of SQMC. We first introduce the model and the notations we consider in this work and then give a short description of SQMC. A new consistency result for the forward step is presented, which has the advantage to rely on weaker assumptions. Finally, this section provides new results on low discrepancy point sets with respect to non uniform distributions that are essential to the analysis of QMC smoothing algorithms. In Section 2.3 we establish the consistency of QMC forward smoothing while our results on QMC

forward-backward smoothing are given Section 2.4. In Section 2.5 we explain how our analysis can be used to derive a QMC version of two filter smoothing and to establish its validity. In Section 2.6 a numerical study examines the performance of the QMC smoothing strategies discussed in this work while Section 2.7 concludes.

2.2 Preliminaries

2.2.1 Model and notations

For ease of notations and following Del Moral (2004) we adopt a Feynman-Kac framework which has the advantage to define the model of interest without writing explicitly its dependence to the observation process $(\mathbf{y}_t)_{t\geq 0}$. More precisely, we consider a generic model for a Markov chain $(\mathbf{x}_t)_{t\geq 0}$ defined on a space $\mathcal{X} \subseteq \mathbb{R}^d$ with initial distribution $m_0(\mathrm{d}\mathbf{x}_0)$ and moving at time $t > 0$ according to a transition kernel $m_t(\mathbf{x}_{t-1}, \mathrm{d}\mathbf{x}_t)$. Let $(G_t)_{t\geq 0}$ be a sequence of potential functions taking their values in $\mathbb{R}^+$. The function G_0 is defined on $\mathcal{X}$ while we assume that, for $t > 0$, G_t is defined on the product space $\mathcal{X} \times \mathcal{X}$. Following Gerber and Chopin (2014) and the standard approach in the QMC literature, we assume in this work that $\mathcal{X} = [0, 1)^d$ (see Gerber and Chopin, 2014, for more details on this point and for how the algorithms proposed below can be amended for unbounded state spaces).

For this Feynman-Kac model $(m_t, G_t)_{t\geq 0}$ we denote by $\overline{\mathbb{Q}}_t(\mathrm{d}\mathbf{x}_t)$ and $\mathbb{Q}_t(\mathrm{d}\mathbf{x}_t)$ two probability measures on $\mathcal{X}$ such that, for any bounded test function $\varphi : \mathcal{X} \to \mathbb{R}$,

$$\overline{\mathbb{Q}}_t(\varphi) = \frac{1}{Z_{t-1}}\mathbb{E}\left[\varphi(\mathbf{x}_t)G_0(\mathbf{x}_0)\prod_{s=1}^{t-1} G_s(\mathbf{x}_{s-1}, \mathbf{x}_s)\right]$$

$$\mathbb{Q}_t(\varphi) = \frac{1}{Z_t}\mathbb{E}\left[\varphi(\mathbf{x}_t)G_0(\mathbf{x}_0)\prod_{s=1}^{t} G_s(\mathbf{x}_{s-1}, \mathbf{x}_s)\right]$$

$$Z_t = \mathbb{E}\left[G_0(\mathbf{x}_0)\prod_{s=1}^{t} G_s(\mathbf{x}_{s-1}, \mathbf{x}_s)\right]$$

and by $\widetilde{\mathbb{Q}}_t(\mathrm{d}\mathbf{x}_{0:t})$ the probability measure on $\mathcal{X}^{t+1}$ such that, for any bounded test function $\varphi : \mathcal{X}^{t+1} \to \mathbb{R}$,

$$\widetilde{\mathbb{Q}}_t(\varphi) = \frac{1}{Z_t}\mathbb{E}\left[\varphi(\mathbf{x}_{0:t})G_0(\mathbf{x}_0)\prod_{s=1}^{t} G_s(\mathbf{x}_{s-1}, \mathbf{x}_s)\right].$$

In the sequel, the notation $0 : t$ is used to denote the set of integers $\{0, \ldots, t\}$ and $\mathbf{x}_{0:t}$ designs the set $\{\mathbf{x}_s\}_{s=0}^t$ of $t + 1$ points in $\mathbb{R}^d$. Similarly, in what follows we use the shorthand $\mathbf{x}^{1:N}$ for the set $\{\mathbf{x}^n\}_{n=1}^N$ of N points in $\mathbb{R}^d$ and $\mathbf{x}_{0:t}^{1:N}$ for the set $\{\mathbf{x}_{0:t}^n\}_{n=1}^N$ of N points in $\mathbb{R}^{(t+1)d}$. Finally, for a probability measure $\pi \in \mathcal{P}(\mathcal{X})$, with

$\mathcal{P}(\mathcal{X})$ the set of probability measures on $\mathcal{X}$ absolutely continuous with respect to the Lebesgue measure, $\pi(\varphi)$ denotes the expectation of $\varphi(\mathbf{x})$ under π.

To make the connection between this Feynman-Kac formulation and state-space models more transparent, let G_t be the density $f^Y(\mathbf{y}_t|\mathbf{x}_t)$, i.e. the density of the law of $\mathbf{y}_t|\mathbf{x}_t$. In this case, the probability measure $\mathbb{Q}_t(\mathrm{d}\mathbf{x}_t)$ is therefore the law of $\mathbf{x}_t|\mathbf{y}_{0:t}$ (i.e. the filtering distribution of $\mathbf{x}_t$), $\overline{\mathbb{Q}}_t(\mathrm{d}\mathbf{x}_t)$ is the law of $\mathbf{x}_t|\mathbf{y}_{0:t-1}$ (i.e. the predictive distribution of $\mathbf{x}_t$) while $\widetilde{\mathbb{Q}}_t(\mathrm{d}\mathbf{x}_{0:t})$ is the object of interest of this work, namely the law of $\mathbf{x}_{0:t}|\mathbf{y}_{0:t}$ (i.e. the smoothing distribution at time t). Finally, note that in this set-up the normalizing constant Z_t is the likelihood function computed from the set of $t+1$ observations $\mathbf{y}_{0:t}$.

In order to establish consistency results for QMC forward-backward smoothing we need a suitable metric. As in Gerber and Chopin (2014), our results are stated in term of the *extreme* norm, defined, for two probability measures π_1 and π_2 on $[0,1)^d$, by

$$\|\pi_1 - \pi_2\|_{\mathrm{E}} = \sup_{B \in \mathcal{B}_{[0,1)^d}} |\pi_1(B) - \pi_2(B)|$$

where $\mathcal{B}_{[0,1)^d} = \{B = \prod_{i=1}^d [a_i, b_i],\ 0 \leq a_i < b_i < 1\}$. The extreme norm is natural in QMC contexts since it can be viewed as the generalization of the *extreme discrepancy* of a point set $\mathbf{u}^{1:N}$ in $[0,1)^d$, defined by

$$D(\mathbf{u}^{1:N}) = \|\mathcal{S}(\mathbf{u}^{1:N}) - \lambda_d\|_{\mathrm{E}}$$

where λ_d denotes the Lebesgue measure on $\mathbb{R}^d$ and $\mathcal{S}$ is the operator that associates to the point set $\mathbf{u}^{1:N}$ its empirical distribution $N^{-1}\sum_{n=1}^N \delta_{\mathbf{u}^n}$. The extreme discrepancy therefore measures how a point set spreads evenly over $[0,1)^d$ and is used to define formally QMC point sets. To be more specific, $\mathbf{u}^{1:N}$ is a QMC point set in $[0,1)^d$ if $D(\mathbf{u}^{1:N}) = \mathcal{O}(N^{-1}(\log N)^d)$. Note that, for a sample $\mathbf{u}^{1:N}$ of N IID uniform random numbers in $[0,1)^d$, $D(\mathbf{u}^{1:N}) = \mathcal{O}(N^{-1/2}\log\log N)$ almost surely by the law of iterated logarithm (see e.g. Niederreiter, 1992, page 167). There exists many constructions of QMC point sets in the literature (see Niederreiter, 1992; Dick and Pillichshammer, 2010, or more details on this topic) and, although we write $\mathbf{u}^{1:N}$ rather than $\mathbf{u}^{N,1:N}$, $\mathbf{u}^{1:N}$ may not necessarily be the N first points of a fixed sequence, i.e. one may have $\mathbf{u}^{N,N-1} \neq \mathbf{u}^{N-1,N-1}$. However, it is worth keeping in mind that all the results presented below hold both for point sets and sequences.

Even if in this work we are mainly interested in consistency results, we will sometimes talk about randomized QMC (RQMC) point sets. Formally, $\mathbf{u}^{1:N}$ is RQMC point set if it is a QMC point set with probability one and if, marginally, $\mathbf{u}^n \sim \mathcal{U}([0,1)^d)$ for all $n \in 1:N$.

The last notation we introduce at this stage concerns the Hilbert space filling curve which plays a key role in the construction and the analysis of SQMC. The Hilbert curve $H : [0,1] \to [0,1]^d$ is a Hölder continuous fractal map that fills completely $[0,1]^d$ (see Appendix A for a presentation of the mains properties of H). In what

follows, we denote by $h : [0,1]^d \to [0,1]$ its pseudo-inverse which verifies, for any $\mathbf{x} \in [0,1]^d$, $H \circ h(\mathbf{x}) = \mathbf{x}$, and, for $d = 1$, we use the natural convention that H and h are the identity mappings, i.e. $H(x) = h(x) = x$, $\forall x \in [0,1]$. It is worth noting that the Hilbert curve is note unique and, in this work, we assume that H is such that $H(0) = \mathbf{0} \in [0,1]^d$ (this is in fact the classical way to construct the Hilbert curve, see e.g. Hamilton and Rau-Chaplin, 2008). This technical assumption is needed in order to be consistent with the fact that we work with left-closed and right-opened hypercubes since, in that case, $h([0,1)^d) = [0,1)$.

2.2.2 Quasi-Monte Carlo filtering

Sequential Monte Carlo, or particle filtering, is a class of iterative algorithms that use resampling and mutation steps to move from a discrete approximation $\widehat{\mathbb{Q}}_t^N(\mathrm{d}\mathbf{x}_t)$ of $\mathbb{Q}_t(\mathrm{d}\mathbf{x}_t)$ to an approximation $\widehat{\mathbb{Q}}_{t+1}^N(\mathrm{d}\mathbf{x}_{t+1})$ of $\mathbb{Q}_{t+1}(\mathrm{d}\mathbf{x}_{t+1})$ (see Algorithm 2.1 and Theorem 2.1 below for a precise definition of $\widehat{\mathbb{Q}}_t^N$). Informally, the resampling step amounts to sample from the discrete distribution $\widehat{\mathbb{Q}}_t^N(\mathrm{d}\mathbf{x}_t)$ to get an unweighted sample which is approximatively distributed according to $\mathbb{Q}_t(\mathrm{d}\mathbf{x}_t)$. Next, in the mutation step, the Markov kernel $m_{t+1}(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t+1})$ is used to generate new particles which produce an unweighted sample targeting $\overline{\mathbb{Q}}_{t+1}(\mathrm{d}\mathbf{x}_{t+1})$. Finally, we assign to each particle a weight proportional to the potential function so that the resulting weighted sum of dirac measures, denoted by $\widehat{\mathbb{Q}}_{t+1}^N(\mathrm{d}\mathbf{x}_{t+1})$, provides an approximation of $\mathbb{Q}_{t+1}(\mathrm{d}\mathbf{x}_{t+1})$.

The basic objective of SQMC is to replace at each time step all the uniform pseudo-random numbers used in a standard particle filter algorithm by a QMC point set $\mathbf{u}_t^{1:N}$ of appropriate dimension. In the deterministic version of SQMC, the only known properties of $\mathbf{u}_t^{1:N}$ is that its discrepancy converges to zero as N goes to infinity. Intuitively, it is therefore clear that to get a consistent algorithm we need to transform the QMC point sets in a way which preserves the consistency in the sense of the extreme norm. Formally, if we have a target distribution π and a point set $\mathbf{u}^{1:N}$ such that $D(\mathbf{u}^{1:N}) \to 0$ as $N \to +\infty$, we need a transformation Γ_π such that $\|\Gamma_\pi(\mathbf{u}^{1:N}) - \pi\|_{\mathrm{E}} \to 0$ as $N \to +\infty$. Based on an idea first studied by Hlawka and Mück (1972), Gerber and Chopin (2014) propose to use the inverse of the Rosenblatt transformation (Rosenblatt, 1952) F_π of π, defined through the following chain rule decomposition:

$$F_\pi(\mathbf{x}) = \left(F_{\pi,1}(x_1), F_{\pi,2}(x_2|x_1), \ldots, F_{\pi,d}(x_d|x_{1:d-1})\right)^T, \quad \mathbf{x} = (x_1, \ldots, x_d)^T \in \mathcal{X},$$

where $F_{\pi,1}$ is the CDF of the marginal distribution of the first component (relative to π), and for $i \geq 2$, $F_{\pi,i}(\cdot|x_{1:i-1})$ is the CDF of component x_i, conditional on $(x_1, \ldots, x_{i-1})$, again relative to π.

The main difficulty of this approach comes from the fact that $\widehat{\mathbb{Q}}_t^N(\mathrm{d}\mathbf{x}_t)$ is a multivariate discrete distribution and therefore we can not invert its Rosenblatt

Algorithm 2.1 SQMC Algorithm

Operations must be performed for all $n \in 1:N$
set $t = 0$
for $t = 0$ **do**
  Generate a QMC point set $\mathbf{u}_0^{1:N}$ in $[0,1)^d$, and compute $\mathbf{x}_0^n = F_{m_0}^{-1}(\mathbf{u}_0^n)$
  Compute $W_0^n = G_0(\mathbf{x}_0^n)/\sum_{m=1}^N G_0(\mathbf{x}_0^m)$
  $t \leftarrow t+1$
end for
while $t \leq T$ **do**
  Generate a QMC point set $\mathbf{u}_t^{1:N}$ in $[0,1)^{d+1}$, let $\mathbf{u}_t^n = (u_t^n, \mathbf{v}_t^n)$
  Find permutation τ such that $u_t^{\tau(1)} \leq \ldots \leq u_t^{\tau(N)}$
  Hilbert sort: find permutation σ_{t-1} such that $h(\mathbf{x}_{t-1}^{\sigma_{t-1}(1)}) \leq \ldots \leq h(\mathbf{x}_{t-1}^{\sigma_{t-1}(N)})$
  Compute $a_{t-1}^n = F_{t,N}^{-1}(u_t^{\tau(n)})$ where, $F_{t,N}(m) = \sum_{i=1}^N W_{t-1}^{\sigma_{t-1}(i)} \mathbb{I}(i \leq m)$
  Compute $\mathbf{x}_t^n = F_{m_t}^{-1}(\hat{\mathbf{x}}_{t-1}^n, \mathbf{v}_t^{\tau(n)})$ where $\hat{\mathbf{x}}_{t-1}^n = \mathbf{x}_{t-1}^{a_{t-1}^n}$
  Compute $W_t^n = G_t(\hat{\mathbf{x}}_{t-1}^n, \mathbf{x}_t^n)/\sum_{m=1}^N G_t(\hat{\mathbf{x}}_{t-1}^m, \mathbf{x}_t^m)$
  $t \leftarrow t+1$
end while

transformation. The idea developed in Gerber and Chopin (2014) to overcome this problem is to "project" the nodes of $\widehat{\mathbb{Q}}_t^N(\mathrm{d}\mathbf{x}_t)$ into $[0,1)$ using the pseudo-inverse of the Hilbert space filling curve. The inverse Rosenblatt transformation (i.e. the generalized inverse CDF) of the resulting distribution $\widehat{\mathbb{Q}}_{t,h}^N(\mathrm{d}h_t)$ can be used to generate a point set $\hat{h}_t^{1:N}$ in $[0,1)$ which is then projected back into $[0,1)^d$ using the Hilbert curve, yielding an unweighed point set $\hat{\mathbf{x}}_t^{1:N}$. Finally, in the mutation step, we move each particle $\hat{\mathbf{x}}_t^n$ using $F_{m_t}^{-1}(\hat{\mathbf{x}}_t^n, \cdot)$, the inverse Rosenblatt transformation of the distribution $m_{t+1}(\hat{\mathbf{x}}_t^n, \mathrm{d}\mathbf{x}_{t+1})$. These steps are summarized in Algorithm 2.1.

The consistency of Algorithm 2.1 for the extreme metric is established in Gerber and Chopin (2014, Theoem 5). Theorem 2.1 below provides a slightly different version of this result which only assumes that $F_{m_t}(\mathbf{x}_{t-1}, \mathbf{x}_t)$ is Hölder (instead of Lipschitz) continuous on $[0,1)^{2d}$. As we will see, Hölder continuity is also the right degree of smoothness for the backward step of SQMC. In addition, Theorem 2.1 allows us to recall the assumptions that underpin SQMC. For convenience, let $F_{m_t}(\mathbf{x}_{t-1}, \mathbf{x}_t) = F_{m_0}(\mathbf{x}_0)$ in the statement of Theorem 2.1 when $t = 0$. Also, for a probability measure $\pi \in \mathcal{P}([0,1)^{d_1})$ and a kernel $K : [0,1)^{d_1} \to \mathcal{P}([0,1)^{d_2})$, we write $\pi \otimes K(\mathrm{d}(\mathbf{x}_1, \mathbf{x}_2))$ the probability measure $\pi(\mathrm{d}\mathbf{x}_1)K(\mathbf{x}_1, \mathrm{d}\mathbf{x}_2)$ on $[0,1)^{d_1+d_2}$.

Theorem 2.1. *Consider the set-up of Algorithm 2.1 where, for all $t \in 0:T$, $(\mathbf{u}_t^{1:N})_{N\geq 1}$ is a sequence of point sets in $[0,1)^{d_t}$, with $d_0 = d$ and $d_t = d+1$ for $t > 0$, such that $D(\mathbf{u}_t^{1:N}) \to 0$ as $N \to +\infty$. Assume the following holds for all $t \in 0:T$:*

1. *The components of $\mathbf{x}_t^{1:N}$ are pairwise distinct, $\mathbf{x}_t^n \neq \mathbf{x}_t^m$ for $n \neq m$;*

2. *G_t is continuous and bounded;*

3. *$F_{m_t}(\mathbf{x}_{t-1}, \mathbf{x}_t)$ is such that*

   (a) *For $i \in 1:d$ and for a fixed $\mathbf{x}'$, the i-th coordinate of $F_{m_t}(\mathbf{x}', \mathbf{x})$ is strictly increasing in $x_i \in [0,1)$;*

   (b) *Viewed as a function of $\mathbf{x}'$ and $\mathbf{x}$, $F_{m_t}(\mathbf{x}', \mathbf{x})$ is Hölder continuous;*

   (c) *For $i \in 1:d$, $m_{ti}(\mathbf{x}', x_{1:i-1}, \mathrm{d}x_i)$, the distribution of the component x_i conditional on $(x_1, .., x_{i-1})$ relative to $m_t(\mathbf{x}', \mathrm{d}\mathbf{x})$, admits a density $p_{ti}(x_i | x_{1:i-1}, \mathbf{x}')$ with respect to the Lebesgue measure such that $\|p_{ti}(\cdot|\cdot)\|_\infty < +\infty$.*

4. *$\mathbb{Q}_t(\mathrm{d}\mathbf{x}_t) = p_t(\mathbf{x}_t)\lambda_d(\mathrm{d}\mathbf{x}_t)$ where $p_t(\mathbf{x}_t)$ is a strictly positive bounded density.*

For $t \in 0:T$, let $\widehat{\mathbb{Q}}_t^N(\mathrm{d}\mathbf{x}_t) = \sum_{n=1}^N W_t^n \delta_{\mathbf{x}_t^n}(\mathrm{d}\mathbf{x}_t)$ and, for $t \in 1:T$, let $P_{t,h}^N = (h(\hat{\mathbf{x}}_{t-1}^{1:N}), \mathbf{x}_t^{1:N})$ and $m_{t,h}(h_{t-1}, \mathrm{d}\mathbf{x}_t) = m_t(H(h_{t-1}), \mathrm{d}\mathbf{x}_t)$. Then, under Assumptions 1-4, we have, for $t \in 1:T$,

$$\left\| \mathcal{S}(P_{t,h}^N) - \mathbb{Q}_{t-1,h} \otimes m_{t,h} \right\|_{\mathrm{E}} \to 0, \quad \text{as } N \to +\infty$$

and, for $t \in 0:T$,

$$\|\widehat{\mathbb{Q}}_t^N - \mathbb{Q}_t\|_{\mathrm{E}} \to 0, \quad \text{as } N \to +\infty.$$

The difference with Gerber and Chopin (2014, Theorem 5) is Assumption 3, where 3c was not needed but it was assumed that F_{m_t} is a Lipschitz function. In this work, Assumption 3c will be required to establish the validity of the backward step. Assumption 1 is a technical condition that is verified almost surely for the randomized version of SQMC while assuming that G_t is bounded is standard in particle filtering (Del Moral, 2004).(e.g. one may have $\mathbf{x}_{N+1}^n \neq \mathbf{x}_N^n$). In our notations, we drop the dependence of point sets on N, i.e. we write $(\mathbf{x}^{1:N})_{N\geq 1}$ rather than $(\mathbf{x}^{N,1:N})_{N\geq 1}$, although in full generality $\mathbf{x}^{1:N}$ may not necessarily be the N first points of a fixed sequence.

The proof of Theorem 2.1 is omitted since it can be directly deduced from the proof of Gerber and Chopin (2014, Theorem 5) and from the generalization of the result of Hlawka and Mück (1972, "Satz 2") presented in the next subsection, which constitutes one of the key ingredients to study the backward pass of SQMC.

2.2.3 A generalization of Hlawka and Mück (1972, "Satz 2")

Theorem 2.2 generalizes Hlawka and Mück (1972, "Satz 2") to the case where point sets in $[0,1)^d$ are transformed through a Hölder continuous Rosenblatt transformation, while Hlawka and Mück (1972, "Satz 2") relies on a Lipschitz assumption (see Appendix B.1 for a proof).

Theorem 2.2. *Let π be a probability measure on $[0,1)^d$ and assume the following:*

1. *Viewed as a function of $\mathbf{x}$, $F_\pi(\mathbf{x})$ is Hölder continuous with Hölder exponent $\kappa \in (0,1]$;*
2. *For $i \in 1:d$, the i-th coordinate of $F_\pi(\mathbf{x})$ is strictly increasing in $x_i \in [0,1)$;*
3. *For $i \in 1:d$, $\pi_i(x_{1:i-1}, \mathrm{d}x_i)$, the distribution of the component x_i conditional on $(x_1, .., x_{i-1})$ relative to $\pi(\mathrm{d}\mathbf{x})$, admits a density $p_i(x_i|x_{1_{i-1}})$ with respect to the Lebesgue measure such that $\|p_i(\cdot|\cdot)\|_\infty < +\infty$.*

Let $\mathbf{u}^{1:N}$ be a point set in $[0,1)^d$ and, for $n \in 1:N$, define $\mathbf{x}^n = F_\pi^{-1}(\mathbf{u}^n)$. Then, for a constant $c > 0$,

$$\|\mathcal{S}(\mathbf{x}^{1:N}) - \pi\|_{\mathrm{E}} \leq cD(\mathbf{u}^{1:N})^{1/\tilde{d}}$$

where $\tilde{d} = \sum_{i=0}^{d-1} \lceil \kappa^{-1} \rceil^i$.

Note that, when the Rosenblatt transformation F_π is Lipschitz, $\tilde{d} = d$ and therefore we recover the result given in Hlawka and Mück (1972). In this case, Assumption 3 is not needed. Also, it is worth remarking that the rate provided in Theorem 2.2 decreases quickly as the Hölder exponent κ decreases. For instance, if $\kappa = 1/2$, the convergence rate is of order $\mathcal{O}(D(\mathbf{u}^{1:N})^{1/2^d-1})$ and hence is very slow even for moderated values of d.

In what follows we will not directly use Theorem 2.2. Rather, as Hlawka and Mück (1972, "Satz 2") is the starting point for the consistency results of SQMC, Theorem 2.2 is the starting point to establish the consistency of the QMC forward-backward algorithm (see Theorem 2.3 below) because it turns out that the backward step of SQMC amounts to transform a QMC point set in $[0,1)^{T+1}$ using the inverse Rosenblatt transformation of a discrete distribution (see Section 2.4.2) that behaves "as if" it was $(1/d)$-Hölder continuous.

If Theorem 2.2 could have been omitted (or hidden in the proofs) we have decided to present it because it is interesting in itself. Indeed, the construction of low discrepancy point sets with respect to non uniform distributions is an important problem that is motivated by the generalized Koksma-Hlawka inequality (Aistleitner and Dick, 2014, Theorem 1):

$$\left| \frac{1}{N} \sum_{n=1}^{N} \varphi(\mathbf{x}^n) - \int_{[0,1)} \varphi(\mathbf{x}) \pi(\mathrm{d}\mathbf{x}) \right| \leq V(\varphi) \|\mathcal{S}(\mathbf{x}^{1:N}) - \pi\|_{\mathrm{E}}$$

where $V(\varphi)$ is the variation of φ in the sense of Hardy and Krause. It is also interesting to mention that the inverse Rosenblatt transformation is the best known construction of low discrepancy point sets for non uniform probability measures, although the bounds for the extreme metric given in Hlawka and Mück (1972, "Satz 2") and in Theorem 2.2 are very far from the best known achievable rate

since Aistleitner and Dick (2013, Theorem 1) establish the existence, for any probability measure π on $[0,1)^d$, of a sequence $(\mathbf{x}^n)_{n\geq 1}$ verifying $\|\mathcal{S}(\mathbf{x}^{1:N}) - \pi\|_{\mathrm{E}} = \mathcal{O}(N^{-1}(\log N)^{0.5(3d+1)})$.

2.2.4 Discrepancy conversion through the Hilbert space filling curve

At this point it worth noting that to obtain the consistency of SQMC (Algorithm 2.1) it was not needed to show that a low discrepancy point set in $[0,1)$ remains a low discrepancy point set in $[0,1)^d$ once transformed through H. Indeed, at time $t > 1$ we map the particles $\mathbf{x}_{t-1}^{1:N}$ into $[0,1)$ using h and resample them for the sole purpose of generating new particles $\mathbf{x}_t^{1:N}$. In particular, we do not care about the discrepancy properties of the "resampled" point set $\hat{\mathbf{x}}_{t-1}^{1:N}$ since, to establish the consistency of SQMC, we only need that $P_{t,h}^N$ has low discrepancy with respect to the proposal distribution $\mathbb{Q}_{t-1,h} \otimes m_{t,h}$, as outlined in the statement of Theorem 2.1.

In contrast, and as it will become clear in the next subsection (see also Section 2.4.3), the estimation of the smoothing distribution $\widetilde{\mathbb{Q}}_T(\mathrm{d}\mathbf{x}_{0:T})$ requires that transformations through the Hilbert curve preserve the consistency for the extreme metric. The following theorem provides a general result concerning the conversion of discrepancies through H that will be essential to establish the consistency of the backward pass of SQMC (Theorem 2.3 below). See also He and Owen (2014) for results concerning the conversion through H of low discrepancy point sets with respect to the uniform distribution on $[0,1)$.

Theorem 2.3. *Let $\pi(\mathrm{d}\mathbf{x}) = \pi(\mathbf{x})\mathrm{d}\mathbf{x}$ be a probability measure on $[0,1)^d$ with bounded density π, π_h be the image of π by h and $(\pi_h^N)_{N\geq 1}$ be a sequence of probability measures on $[0,1)$ such that $\|\pi_h^N - \pi_h\|_{\mathrm{E}} \to 0$ as $N \to +\infty$ for a probability distribution π_h on $[0,1)$. Let π^N and π be, respectively, the image by H of π_h^N and π_h. Then, for all $N \geq 1$,*

$$\|\pi^N - \pi\|_{\mathrm{E}} \leq c\|\pi_h^N - \pi_h\|_{\mathrm{E}}^{1/d}$$

for a constant $c > 0$.

See Appendix B.2 for a proof.

As a corollary, note that, under the assumptions of Theorem 2.1, the point set $P_t^N = (\hat{\mathbf{x}}_{t-1}^{1:N}, \mathbf{x}_t^{1:N})$ is such that, as $N \to +\infty$,

$$\|\mathcal{S}(P_t^N) - \mathbb{Q}_{t-1} \otimes m_t\|_{\mathrm{E}} \to 0.$$

This result follows from the next corollary (see Appendix B.3 for a proof).

Corollary 2.1. *Let $K : [0,1)^d \to \mathcal{P}([0,1)^s)$ be a Markov kernel, $K_h(h_1, \mathrm{d}\mathbf{x}_2) = K(h(\mathbf{x}_1), \mathrm{d}\mathbf{x}_2)$ and $P_h^N = (h_1^{1:N}, \mathbf{x}_2^{1:N})$ be a sequence of point sets in $[0,1)^{1+s}$ such*

that, as $N \to +\infty$, $\|\mathcal{S}(P_h^N) - \pi_h \otimes K_h\|_{\mathrm{E}} \to 0$. *Let* $P^N = \left(H(h_1^{1:N}), \mathbf{x}_2^{1:N}\right)$. *Then, for all* $N \geq 1$,

$$\|\mathcal{S}(P^N) - \pi^N \otimes K\|_{\mathrm{E}} \leq c\|\mathcal{S}(P_h^N) - \pi_h \otimes K_h\|_{\mathrm{E}}^{1/d}$$

for the same constant c *as in Theorem 2.3.*

A direct consequence of this observation is that Algorithm 2.1 can be trivially adapted to carry out forward the estimation of the smoothing distribution, as briefly explained in the next section.

2.3 Quasi-Monte Carlo forward smoothing

Consider now Algorithm 2.1 where, at iteration t, the Hilbert sort step is replaced by the following one:

Hilbert sort: find permutation σ_{t-1} such that $h^t(\mathbf{x}_{0:t-1}^{\sigma_{t-1}(1)}) \leq \ldots \leq h^t(\mathbf{x}_{0:t-1}^{\sigma_{t-1}(N)})$

with h^t the inverse of a Hilbert curve H^t that maps $[0,1]$ into $[0,1]^{dt}$. For $t \in 1:T$, let $\mathbf{z}_{t-1} = \mathbf{x}_{0:t-1}$, $\hat{\mathbf{z}}_{t-1}^n = \mathbf{z}_{t-1}^{a_{t-1}^n}$ and $\mathbf{z}_t^n = (\hat{\mathbf{z}}_{t-1}^n, \mathbf{x}_t^n)$, $n \in 1:N$. We now show that, at time $t \geq 0$, the resulting algorithm provides a weighted sample $(W_t^{1:N}, \mathbf{z}_t^{1:N})$ such that

$$\left\| \sum_{n=1}^N W_t^n \delta_{\mathbf{z}_t^n} - \widetilde{\mathbb{Q}}_t \right\|_{\mathrm{E}} \to 0, \quad \text{as } N \to +\infty \tag{2.29}$$

where we recall that $\widetilde{\mathbb{Q}}_t$ denotes the smoothing distribution at time t.

To see this, let $\widetilde{\mathbb{Q}}_{t-1,h^t}$ be the image by h^t of $\widetilde{\mathbb{Q}}_{t-1}$ and $\tilde{P}_{t,h^t}^N = \left(h^t(\hat{\mathbf{z}}_{t-1}^{1:N}), \mathbf{x}_t^{1:N}\right)$. Then, replacing Assumption 4 of Theorem 2.1 by

> *4'.* $\widetilde{\mathbb{Q}}_t(\mathrm{d}\mathbf{z}_t) = \tilde{p}_t(\mathbf{z}_t)\lambda_{d(t+1)}(\mathrm{d}\mathbf{z}_t)$ *where* $\tilde{p}_t(\mathbf{z}_t)$ *is a strictly positive bounded density*

we get $\|\mathcal{S}(\tilde{P}_{t,h^t}^N) - \widetilde{\mathbb{Q}}_{t-1,h^t} \otimes m_{t,h}\|_{\mathrm{E}} \to 0$ as $N \to +\infty$. Therefore, by Corollary 2.1,

$$\|\mathcal{S}(\mathbf{z}_t^{1:N}) - \widetilde{\mathbb{Q}}_{t-1} \otimes m_t\|_{\mathrm{E}} \to 0, \quad \text{as } N \to +\infty. \tag{2.30}$$

Finally, since the Radon-Nikodym derivative

$$G_t(\mathbf{x}_{t-1}, \mathbf{x}_{t-1}) \propto \frac{\widetilde{\mathbb{Q}}_t}{\widetilde{\mathbb{Q}}_{t-1} \otimes m_t}(\mathrm{d}(\mathbf{x}_{0:t-1}, \mathbf{x}_t)),$$

is continuous and bounded, Gerber and Chopin (2014, Theorem 1), together with (2.30), implies (2.29).

This result on QMC forward smoothing is presented for sake of completeness but it is clear that it is of little practical interest. Indeed, in empirical works, T is typically large so that transformations through H^t will lead to poor convergence rates, as shown in Theorem 2.3. In addition, as for its classical Monte Carlo counterpart, QMC forward smoothing is subject to weight degeneracy problems and is therefore not suitable for efficient estimation of the smoothing distribution, contrary to the smoothing techniques we discuss below.

2.4 Quasi-Monte Carlo backward smoothing

We now turn to the analysis of QMC forward-backward smoothing algorithms. As a preliminary result, we start by showing that the estimate of the filtering distribution $\mathbb{Q}_t(\mathrm{d}\mathbf{x}_t)$ obtained at each time step from Algorithm 2.1 can be merged together using the backward decomposition of the smoothing distribution (Del Moral et al., 2010) to build an estimate $\widetilde{\mathbb{Q}}_T^N(\mathrm{d}\mathbf{x}_{0:T})$ that is consistent for the extreme metric.

2.4.1 Backward decomposition

We assume from now on that $m_t(\mathbf{x}_{t-1}, \mathrm{d}\mathbf{x}_t) = m_t(\mathbf{x}_{t-1}, \mathbf{x}_t)\lambda_d(\mathrm{d}\mathbf{x}_t)$ where $m_t(\cdot,\cdot) > 0$. The backward decomposition of the smoothing distribution is given by (Del Moral et al., 2010):

$$\widetilde{\mathbb{Q}}_T(\mathrm{d}\mathbf{x}_{0:T}) = \mathbb{Q}_T(\mathrm{d}\mathbf{x}_T) \prod_{t=1}^{T} \mathcal{M}_{t,\mathbb{Q}_{t-1}}(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t-1}) \tag{2.31}$$

where, for any $\pi \in \mathcal{P}([0,1)^d)$ and $t \in 1:T$, $\mathcal{M}_{t,\pi} : [0,1)^d \to \mathcal{P}([0,1)^d)$ is a Markov kernel such that

$$\mathcal{M}_{t,\pi}(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t-1}) = \frac{m_t(\mathbf{x}_{t-1}, \mathbf{x}_t)}{\pi(m_t)(\mathbf{x}_t)} \pi(\mathrm{d}\mathbf{x}_{t-1}).$$

The following theorem shows that the SQMC plug-in estimates $\widetilde{\mathbb{Q}}_T^N$ of $\widetilde{\mathbb{Q}}_T$, obtained by replacing $\mathbb{Q}_t$ by the SQMC estimate $\widehat{\mathbb{Q}}_t^N$ in (2.31), is consistent for the extreme norm (see Appendix C for a proof).

Theorem 2.1. *Consider the set-up of Algorithm 2.1. Assume that the assumptions of Theorem 2.1 hold and that $m_t(\mathbf{x}_{t-1}, \mathrm{d}\mathbf{x}_t) = m_t(\mathbf{x}_{t-1}, \mathbf{x}_t)\lambda_d(\mathrm{d}\mathbf{x}_t)$ where $m_t(\cdot,\cdot) > 0$ for all $t \in 1:T$* (Assumption (H1)). *For $t \in 1:T$, define*

$$\widetilde{\mathbb{Q}}_t^N(\mathrm{d}\mathbf{x}_{0:t}) = \widehat{\mathbb{Q}}_t^N(\mathrm{d}\mathbf{x}_t) \prod_{s=1}^{t} \mathcal{M}_{s,\widehat{\mathbb{Q}}_{s-1}^N}(\mathbf{x}_s, \mathrm{d}\mathbf{x}_{s-1})$$

and let $\tilde{G}_t(\mathbf{x}_{t-1}, \mathbf{x}_t) = \frac{m_t(\mathbf{x}_{t-1}, \mathbf{x}_t)}{\mathbb{Q}_{t-1}(m_t)(\mathbf{x}_t)}$.

1. *For all $t \in 1:T$, assume that $\tilde{G}_t(\cdot, \mathbf{x}_t)$ is continuous with $\|\tilde{G}_t\|_\infty < +\infty$* (Assumption (H2)). *Then, for all $t \in 1:T$,*

$$\sup_{\mathbf{x}_t \in [0,1)^d} \|\mathcal{M}_{t,\widehat{\mathbb{Q}}_{t-1}^N}(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t-1}) - \mathcal{M}_{t,\mathbb{Q}_{t-1}}(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t-1})\|_{\mathrm{E}} \to 0, \quad \text{as } N \to +\infty. \tag{2.32}$$

2. *For all $t \in 1:T$, assume that $F_{\mathcal{M}_{t,\mathbb{Q}_{t-1}}}(\mathbf{x}_t, \mathbf{x}_{t-1})$ satisfies Assumptions 3a and 3b of Theorem 2.1* (Assumption (H3)), *and that* (2.32) *holds. Then, for all $t \in 1:T$,*

$$\|\widetilde{\mathbb{Q}}_t^N - \widetilde{\mathbb{Q}}_t\|_{\mathrm{E}} \to 0, \quad \text{as } N \to +\infty. \tag{2.33}$$

The assumptions on $\{\tilde{G}_t\}_{t=1}^T$ in the first part of the theorem are natural since, as we will see below, $\{\tilde{G}_t\}_{t=1}^T$ play the role of importance sampling weights in the backward step while the Hölder assumption for the Rosenblatt transformation $F_{\mathcal{M}_t,\mathbb{Q}_{t-1}}$ comes from Gerber and Chopin (2014, Lemma 10). The result given in the first part of the theorem has no particular meaning at this stage but will be essential to establish the consistency of the backward pass of SQMC.

2.4.2 Backward step of SQMC

The backward step of SQMC as proposed in Gerber and Chopin (2014) is recalled in Algorithm 2.2.

Before proposing asymptotic results for this QMC forward-backward algorithm it is worth noting that Algorithm 2.2 works very similarly as in standard Monte Carlo settings because the particles are already sorted according to their Hilbert index in the forward step (Algorithm 2.1). In fact, the only difference is that a QMC point set in $[0,1)^{T+1}$ is used rather than a set of pseudo-random numbers.

To understand intuitively why this SQMC backward pass is valid to sample from the smoothing distribution, note that Algorithm 2.2 proceeds in reality in two steps. First, it generates $\tilde{h}_{0:T}^{1:N}$, a point set in $[0,1)^{T+1}$ obtained using the inverse Rosenblatt transformation of the image by the mapping $h_T : (\mathbf{x}_0, \ldots, \mathbf{x}_T) \mapsto (h(\mathbf{x}_0), \ldots . h(\mathbf{x}_T))$ of $\widetilde{\mathbb{Q}}_T^N(\mathrm{d}\mathbf{x}_{0:T})$, which is given by

$$\widetilde{\mathbb{Q}}_{T,h_T}^N(\mathrm{d}h_{0:T}) := \widehat{\mathbb{Q}}_{T,h}^N(\mathrm{d}h_T) \prod_{t=1}^T \mathcal{M}_{t,\widehat{\mathbb{Q}}_{t-1,h}^N}^h(h_t, \mathrm{d}h_{t-1}) \tag{2.35}$$

where we recall that $\widehat{\mathbb{Q}}_{t,h}^N$ is the image of $\widehat{\mathbb{Q}}_t^N$ by h and where, for any $\pi \in \mathcal{P}([0,1))$ and $t \in 1:T$, $\mathcal{M}_{t+1,\pi}^h : [0,1) \to \mathcal{P}([0,1))$ is a Markov kernel such that

$$\mathcal{M}_{t,\pi}^h(h_t, \mathrm{d}h_{t-1}) = \frac{m_t(H(h_t), H(h_{t-1}))}{\pi(m_t)(H(h_t))} \pi(\mathrm{d}h_{t-1}).$$

Algorithm 2.2 Backward step of SQMC

Input: $\mathbf{x}_{0:T}^{\sigma_{0:T}(1:N)}$ and $W_{0:T}^{\sigma_{0:T}(1:N)}$ (output of Algorithm 2.1 after the Hilbert sort step, i.e for all $t \in 0:T$, $h(\mathbf{x}_t^{\sigma_t(n)}) \leq h(\mathbf{x}_t^{\sigma_t(m)})$, $n \leq m$) and $\tilde{\mathbf{u}}^{1:N}$ a point set in $[0,1)^{T+1}$

Output: $\tilde{\mathbf{x}}_{0:T}^{1:N}$ (N trajectories in $\mathcal{X}^{T+1}$)

Find permutation τ such that $\tilde{u}_1^{\tau(1)} \leq ... \leq \tilde{u}_1^{\tau(N)}$

For $n \in 1:N$, compute $a_T^n = F_{T,N}^{-1}(u_1^{\tau(n)})$ where $F_{T,N}(m) = \sum_{n=1}^N W_T^{\sigma_T(n)} \mathbb{I}(n \leq m)$

For $n \in 1:N$, set $\tilde{\mathbf{x}}_T^n = \mathbf{x}_T^{a_T^n}$

for $t = T-1 \to 0$ **do**

  for $n = 1 \to N$ **do**

    Set $\tilde{\mathbf{x}}_t^n = \mathbf{x}_t^{\tilde{a}_t^n}$ where $\tilde{a}_t^n = \tilde{F}_{t,N,n}^{-1}(\tilde{u}_{T-1-t+1}^{\tau(n)})$ with

$$\tilde{F}_{t,N,n}(m) = \sum_{i=1}^N \widetilde{W}_t^{\sigma_t(i)}(\tilde{\mathbf{x}}_{t+1}^n) \mathbb{I}(i \leq m)$$

  and, for $i \in 1:N$,

$$\widetilde{W}_t^i(\mathbf{x}_{t+1}) = W_t^i m_{t+1}(\mathbf{x}_t^i, \mathbf{x}_{t+1}) / \left\{ \sum_{k=1}^N W_t^k m_{t+1}(\mathbf{x}_t^k, \mathbf{x}_{t+1}) \right\} \tag{2.34}$$

  end for

end for

Then, Algorithm 2.2 returns $\tilde{\mathbf{x}}_{0:T}^{1:N}$ where $\tilde{\mathbf{x}}_{0:T}^{n} = H_T(\tilde{h}_{0:T}^{n})$ with

$$H_T : (x_0, \ldots, x_T) \in [0,1)^{T+1} \mapsto (H(x_0), \ldots, H(x_T)) \in [0,1)^{d(T+1)}. \tag{2.36}$$

A direct consequence of this inverse Rosenblatt interpretation of the QMC backward step is that, when Algorithm 2.2 uses a RQMC point set as input, the random point $\tilde{\mathbf{x}}_{0:T}^{n}$ is such that, for any function $\varphi : [0,1)^{d(T+1)} \to \mathbb{R}$ and for any $n \in 1:N$, we have $\mathbb{E}[\varphi(\tilde{\mathbf{x}}_{0:T}^{n})|\mathcal{F}_T^N] = \widetilde{\mathbb{Q}}_T^N(\varphi)$, with $\mathcal{F}_T^N$ the σ-algebra generated by the forward step. Together with Theorem 2.1, this observations allows us to deduce the L_2-convergence for test functions φ that are continuous and bounded (see Appendix D for a proof).

Theorem 2.2. *Consider the set-up of the SQMC forward filtering-backward smoothing algorithm (Algorithms 2.1 and 2.2) and assume the following:*

1. *In Algorithm 2.1, $(\mathbf{u}_t^{1:N})_{N\geq 1}$, $t \in 0:T$, are independent random sequences of point sets in $[0,1)^{d_t}$, with $d_0 = d$ and $d_t = d+1$ for $t > 0$, such that, for any $\epsilon > 0$, there exists a $N_{\epsilon,t} > 0$ such that, almost surely, $D(\mathbf{u}_t^{1:N}) \leq \epsilon$, $\forall N \geq N_{\epsilon,t}$;*
2. *In Algorithm 2.2, $(\tilde{\mathbf{u}}^{1:N})_{N\geq 1}$ is a sequence of point sets in $[0,1)^{T+1}$ such that*
   (a) *$\forall n \in 1:N$, $\tilde{\mathbf{u}}^n \sim \mathcal{U}([0,1)^{T+1})$;*
   (b) *For any function $\varphi \in L_2\left([0,1)^{d(T+1)}, \lambda_{d_t}\right)$, $\mathrm{Var}\left(\frac{1}{N}\sum_{n=1}^N \varphi(\mathbf{u}_t^n)\right) \leq C\sigma_\varphi^2 r(N)$ where $\sigma_\varphi^2 = \int \left\{\varphi(\mathbf{u}) - \int \varphi(\mathbf{v})\mathrm{d}\mathbf{v}\right\}^2 \mathrm{d}\mathbf{u}$, and where both C and $r(N)$ do not depend on φ;*
3. *Assumptions H1-H3 of Theorem 2.1 hold.*

Then, for all continuous and bounded function $\varphi : \mathcal{X}^{T+1} \to \mathbb{R}$,

$$\mathbb{E}\left|\mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N})(\varphi) - \widetilde{\mathbb{Q}}_T(\varphi)\right| \to 0, \quad \mathrm{Var}\left(\mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N})(\varphi)\right) \to 0, \quad \text{as } N \to +\infty.$$

Assumption 1 is for instance verified when $\mathbf{u}_t^{1:N}$ are the first N points of a Owen (1995) nested scrambled (t, d_t)-sequence in base $b \geq 2$ (Owen, 1997, 1998). The result is stated for the case where the point sets $\mathbf{u}_t^{1:N}$, $t \in 0:T$, are random but it also holds when deterministic point sets are used as input for the forward pass. In addition, note that this theorem does not assume that the point set used in the backward step has some low discrepancy properties. In particular, Assumption 2 is satisfied with $C = 1$ and $r(N) = N^{-1}$ if $\tilde{\mathbf{u}}^{1:N}$ is a set of $(T+1)$ IID random numbers in $[0,1)^{T+1}$ (see Section 2.4.4 for a discussion one the use of QMC or pseudo-random numbers in the backward step of SQMC).

2.4.3 Consistency of the backward step

Apart from discontinuity problems, it is intuitively more difficult to prove the consistency (for the extreme metric) of the backward step than to prove the consistency of the forward pass of SQMC. First, as Algorithm 2.2 generates a point set $\tilde{h}_{0:T}^{1:N}$ in $[0,1)^{T+1}$ using the inverse Rosenblatt transformation (2.35) and then projects it into the original state space through the mapping H_T, we need to establish that this transformation preserves the low discrepancy properties of $\tilde{h}_{0:T}^{1:N}$.

Second, to prove the consistency of Algorithm 2.1, some smoothness conditions on the Rosenblatt transformation of the Markov kernel $m_{t,h}(h_{t-1}, \mathrm{d}\mathbf{x}_t) = m_t(H(h_{t-1}), \mathrm{d}\mathbf{x}_t)$ was necessary to preserve (in some sense) the low discrepancy properties of the QMC point sets at hand, as explained in Section 2.2.2. Due to the Hölder property of the Hilbert curve, the Hölder continuity of F_{m_t} implies that $F_{m_{t,h}}$ is Hölder continuous as well. Similarly, for the backward step we need assumptions on the Markov kernel $\mathcal{M}_{t+1,\mathbb{Q}_{t-1}}$ which imply sufficient smoothness for the Rosenblatt transformation of $\mathcal{M}^h_{t+1,\widehat{\mathbb{Q}}^N_{t-1,h}}$. Under some conditions, as $N \to +\infty$, this kernel becomes arbitrary close to $\mathcal{M}^h_{t+1,\mathbb{Q}_{t-1,h}}$ and it is therefore clear that we need smoothness conditions on this limiting kernel to establish the validity of Algorithm 2.2. However, this turns out to be a more difficult task than for the forward pass because the two arguments of this kernel are "projections" in $[0,1)$ through the inverse of the Hilbert curve. As shown below, a consistency result for a QMC forward-backward algorithm can be established under a Hölder assumption on the CDF of $\mathcal{M}_{t+1,\mathbb{Q}_{t-1}}$.

In order to focus on these two additional technical difficulties, compared to the SQMC settings, we simplify the analysis by first considering a modified backward step which amount to sample from a continuous distribution, and then show how the result obtain for this latter can be used to provide conditions for the consistency of Algorithm 2.2. The advantage of this approach is that it prevents us to be distracted by complicated discontinuity issues for which we refer to Gerber and Chopin (2014, Theorem 4) for a more elegant solution.

From the discussion of the previous subsection it is natural to consider a backward step which amounts to transform the QMC point set $\tilde{\mathbf{u}}^{1:N}$ in $[0,1)^{T+1}$ through the inverse Rosenblatt transformation of a continuous approximation $\widetilde{\mathbb{Q}}^N_{T,h_T}$ of $\widetilde{\mathbb{Q}}^N_{T,h_T}$. To define $\widetilde{\mathbb{Q}}^N_{T,h_T}$, let $\widehat{\mathbb{Q}}^N_{T,h}$ be the probability measure that corresponds to a continuous approximation of the CDF of $\widehat{\mathbb{Q}}^N_{T,h}$ which is strictly increasing on $[0, h(\mathbf{x}_T^{\sigma_T(N)})]$ with $F_{\widehat{\mathbb{Q}}^N_{T,h}}(h(\mathbf{x}_T^{\sigma_T(N)})) = 1$ and such that, under the assumptions of Theorems 2.1 and 2.1,

$$\|\widehat{\mathbb{Q}}^N_{T,h} - \widehat{\mathbb{Q}}^N_{T,h}\|_{\mathrm{E}} = o(1).$$

Next, for $t \in 1:T$, let $K^N_{t,h}$ be a Markov kernel such that (a) its CDF is continuous on $[0,1) \times [0, h(\mathbf{x}_{t-1}^{\sigma_{t-1}(N)})]$, (b) $\forall h_1 \in [0,1)$, the CDF of $K^N_{t,h}(h_1, \mathrm{d}h_{t-1})$ is strictly

increasing on $[0, h(\mathbf{x}_{t-1}^{\sigma_{t-1}(N)})]$ with $F_{K_{t,h}^N}(h_1, h(\mathbf{x}_{t-1}^{\sigma_{t-1}(N)})) = 1$ and (c)

$$\sup_{h_1 \in [0,1)} \|K_{t,h}^N(h_1, \mathrm{d}h_{t-1}) - \mathcal{M}_{t,\widehat{\mathbb{Q}}_{t-1,h}^N}^h(h_1, \mathrm{d}h_{t-1})\|_{\mathrm{E}} = o(1)$$

under the assumptions of Theorems 2.1 and and 2.1. Finally, we define $\widetilde{\mathbb{Q}}_{T,h_T}^N$ as

$$\widetilde{\mathbb{Q}}_{T,h_T}^N(\mathrm{d}h_{0:T}) := \widehat{\mathbb{Q}}_{T,h}^N(\mathrm{d}h_T) \prod_{t=1}^{T} K_{t,h}^N(h_t, \mathrm{d}h_{t-1})$$

which is, by construction, a continuous distribution on $[0,1)^{T+1}$.

The construction of such a distribution $\widetilde{\mathbb{Q}}_{T,h_T}^N$ is an easy task. For instance, under the assumptions of Theorems 2.1 and 2.1, one can take for $\widehat{\mathbb{Q}}_{T,h}^N$ the probability distribution that corresponds to a linear approximation of the CDF of $\widehat{\mathbb{Q}}_{T,h}^N$ and, similarly, for $h_1 \in [0,1)$, one can construct $K_{t,h}^N(h_1, \mathrm{d}h_{t-1})$ from a linear approximation of the CDF of $\mathcal{M}_{t,\widehat{\mathbb{Q}}_{t-1,h}^N}^h(h_1, \mathrm{d}h_{t-1})$.

The following theorem establishes the consistency of the QMC forward-backward algorithm where in the backward step we transform a QMC point set $\tilde{\mathbf{u}}^{1:N}$ in $[0,1)^{T+1}$ using the (continuous) inverse Rosanblatt transformation of the continuous probability measure $\widetilde{\mathbb{Q}}_{T,h_T}^N$.

Theorem 2.3. *Let $(\tilde{\mathbf{u}}^{1:N})_{N \geq 1}$ be a sequence of point sets in $[0,1)^{T+1}$ such that $D(\tilde{\mathbf{u}}^{1:N}) \to 0$ as $N \to +\infty$. For $n \in 1:N$, let $\check{h}_{0:T}^n = F_{\widetilde{\mathbb{Q}}_{T,h_T}^N}^{-1}(\tilde{\mathbf{u}}^n)$ where $\widetilde{\mathbb{Q}}_{T,h_T}^N$ is as above. Suppose that the Assumptions H1-H3 of Theorem 2.1 hold and that, viewed as a function of $\mathbf{x}_t$ and $\mathbf{x}_{t-1}$, $F_{\mathcal{M}_{t,\mathbb{Q}_{t-1}}}^{cdf}(\mathbf{x}_t, \mathbf{x}_{t-1})$, the CDF of $\mathcal{M}_{t+1,\mathbb{Q}_{t-1}}(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t-1})$, is Hölder continuous for all $t \in 1:T$. Let $\check{\mathbf{x}}_{0:T}^n = H_T(\check{h}_{0:T}^n)$. Then,*

$$\|\mathcal{S}(\check{\mathbf{x}}_{0:T}^{1:N}) - \widetilde{\mathbb{Q}}_T\|_{\mathrm{E}} \to 0 \quad \text{as } N \to +\infty.$$

See Appendix E for a proof.

We are now ready to provide conditions which ensures that QMC forward-backward smoothing (Algorithms 2.1 and 2.2) yields a consistent estimate of the smoothing distribution. The key idea of our consistency result (Corollary 2.1 below) is to show that, for a given point set $\tilde{\mathbf{u}}^{1:N}$, the point set $\tilde{\mathbf{x}}_{0:T}^{1:N}$ generated by Algorithm 2.2 becomes, as N increases, arbitrary close to the point set $\check{\mathbf{x}}_{0:T}^{1:N}$ obtained using the smooth backward step described above.

Corollary 2.1. *Consider the set-up of the SQMC forward filtering-backward smoothing algorithm (Algorithms 2.1 and 2.2) and assume the following:*

1. *$(\tilde{\mathbf{u}}^{1:N})_{N \geq 1}$ is a sequence of point sets in $[0,1)^{T+1}$ such that $D(\tilde{\mathbf{u}}^{1:N}) \to 0$ as $N \to +\infty$;*

2. *Assumptions H1-H3 of Theorem 2.1 hold;*

3. *For all* $t \in 1:T$ $F^{cdf}_{\mathcal{M}_{t,\mathbb{Q}_{t-1}}}(\mathbf{x}_t, \mathbf{x}_{t-1})$ *is Hölder continuous;*

4. *For* $t \in 0:T-1$ *there exists a constant* $c_t > 0$ *such that, for all* $\mathbf{x}_{(t-1):(t+1)} \in \mathcal{X}^3$*,*

$$G_t(\mathbf{x}_{t-1}, \mathbf{x}_t) m_{t+1}(\mathbf{x}_t, \mathbf{x}_{t+1}) \geq c_t;$$

5. *For* $t \in 0:T-1$*,* $m_t(\mathbf{x}_{t-1}, \mathbf{x}_t)$ *is Hölder continuous.*

Then,

$$\|\mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N}) - \widetilde{\mathbb{Q}}_T\|_{\mathrm{E}} \to 0 \quad \text{as } N \to +\infty.$$

See Appendix E.3 for a proof.

Again, at the price of more tedious computations to deal with the discontinuities of Algorithm 2.2, and in the spirit of Gerber and Chopin (2014, Theorem 4), we believe that is possible to weaken the assumptions of Corollary 2.1 and in particular to relax Assumption 4, which essentially implies that the state space $\mathcal{X}$ is compact.

2.4.4 Alternative backward steps

The estimation of the smoothing distribution is a high dimensional problem because the time horizon T is typically large in practice (at least several dozens). Consequently, the interest of using a (R)QMC point set in the backward step may be limited since it is well known that the performance of QMC methods tends to deteriorate as the dimension of the problem at hand increases. For instance, for a QMC quadrature rule on $[0,1)^d$, the error size is typically of order $N^{-\alpha}(\log N)^{\frac{d-1}{2}}$ for a constant $\alpha > 0$ (exceptions to this "rule" are scenarios where the "effective sample" size remains low although d is large, see Glasserman, 2004, p.327, for an example). To address this potential difficulty of QMC in high dimensional settings several authors have proposed to combine QMC points sets and pseudo-random numbers (see Ökten et al., 2006, and references therein). Following this idea, note that the only assumption on $\tilde{\mathbf{u}}^{1:N}$ used in the backward pass is that $D(\tilde{\mathbf{u}}^{1:N})$ goes to zero as N increases. Since point sets of IID uniform random variates verify this condition with probability one, we can therefore approximate the smoothing distribution using (a) SQMC to estimate the filtering distributions for $t \in 0:T$ and (b) a standard Monte Carlo backward smoothing algorithm to estimate $\widetilde{\mathbb{Q}}_T$. Note that using this strategy will obviously result in an estimate which (in the best case) exhibits the $N^{-1/2}$ Monte Carlo convergence rate. However, we can expect, for a given number of particles N, a lower mean square error than for plain Monte Carlo forward-backward smoothing as in the backward step we are sampling from a better approximation of the smoothing distribution.

In practice, we are often interested in evaluating $\widetilde{\mathbb{Q}}_T(\varphi)$ for an additive function $\varphi(\mathbf{x}_{0:T}) = \sum_{t=0}^{T} \varphi_t(\mathbf{x}_t)$. In that case, the suitable QMC backward step is given

in Algorithm 2.3, which at each iteration provides a point set $\bar{\mathbf{x}}_t^{1:N}$ that estimates the marginal smoothing distribution $\widetilde{\mathbb{Q}}_{t|T}(\mathrm{d}\mathbf{x}_t)$. Compared to Algorithm 2.2, this alternative backward pass has the advantage to be based only on QMC point sets of dimension 1, which may be particularly useful when T is large. Indeed, in high dimension the equidistributions properties of QMC point sets deteriorate and become not significantly better than those of Latin hypercube sample. The validity of Algorithm 2.3 to estimate the marginal distribution is a direct consequence of Theorem 2.1, as shown in the next corollary.

Corollary 2.2. *Consider the set-up of Algorithm 2.3 where, for all $t \in 0:T$, $(\bar{u}_t^{1:N})_{N\geq 1}$ is a sequence of point sets in $[0,1)$ such that $D(\bar{u}_t^{1:N}) \to 0$ as $N \to +\infty$. Assume that the assumptions H1-H3 of Theorem 2.1 are verified. Then, for all $t \in 0:T$,*

$$\|\mathcal{S}(\bar{\mathbf{x}}_t^{1:N}) - \widetilde{\mathbb{Q}}_{t|T}\|_{\mathrm{E}} \to 0 \quad \text{as } N \to +\infty.$$

Proof. To prove the result let $\widetilde{\mathbb{Q}}_{t|T}^N(\mathrm{d}\mathbf{x}_t)$ be the marginal distribution of $\mathbf{x}_t$ relative to $\widetilde{\mathbb{Q}}_T^N$ and $\widetilde{\mathbb{Q}}_{t|T,h}^N$ be its image by h. Then, iteration t of Algorithm 2.3 amounts to compute, for $n \in 1:N$, $\bar{\mathbf{x}}_t = H(\bar{h}_t^n)$ where $\bar{h}_t^n = F^{-1}_{\widetilde{\mathbb{Q}}^N_{t|T,h}}(\bar{u}_t^n)$. By Theorem 2.1, $\|\widetilde{\mathbb{Q}}_{t|T}^N - \widetilde{\mathbb{Q}}_{t|T}\|_{\mathrm{E}} \to 0$ as $N \to +\infty$ and therefore, as $\widetilde{\mathbb{Q}}_{t|T}$ admits a bounded density under the assumptions of Theorem 2.1, $\|\widetilde{\mathbb{Q}}_{t|T,h}^N - \widetilde{\mathbb{Q}}_{t|T,h}\|_{\mathrm{E}} \to 0$ (Gerber and Chopin, 2014, Theorem 3). This implies that (Gerber and Chopin, 2014, Theorem 4)

$$\|\mathcal{S}(\bar{h}_t^{1:N}) - \widetilde{\mathbb{Q}}_{t|T,h}\|_{\mathrm{E}} \to 0$$

and therefore the result follows using Theorem 2.3. □

2.5 Two filter smoothing

In this work we focus mainly on consistency results for the backward step of SQMC. However, our analysis may serve to establish the validity of QMC version of other smoothing strategies such as, for instance, two filter smoothing. Two filter smoothing was introduced by Briers et al. (2010) because the forward-backward smoothing algorithm can be subject to degeneracy problem, the reason being that it estimates the smoothing distribution using the particles generated to estimate the filtering distributions. Hence, if $\mathbb{Q}_t(\mathrm{d}\mathbf{x}_t)$ and $\widetilde{\mathbb{Q}}_{t|T}(\mathrm{d}\mathbf{x}_t)$ have high probability mass on different regions of the state space $\mathcal{X}$, a large number of particles is required for the estimates to have a reasonable variance. To solve this issues, Briers et al. (2010) propose to estimate the smoothing distribution using two independent SMC algorithms.

More precisely, two filter smoothing is based on the following decomposition of the smoothing distribution (Briers et al., 2010, Proposition 4), obtained for any

Algorithm 2.3 Backward step of SQMC to target marginal smoothing distributions

Operations must be performed for all $n \in 1:N$.

Input: $\mathbf{x}_{0:T}^{\sigma_t(1:N)}$, $W_{0:T}^{\sigma_t(1:N)}$ (output of Algorithm 2.1 after the Hilbert sort step, i.e for all $t \in 0:T$, $h(\mathbf{x}_t^{\sigma_t(n)}) \leq h(\mathbf{x}_t^{\sigma_t(m)})$, $n \leq m$) and $\bar{u}_{0:T}^{1:N}$, $(T+1)$ point sets in $[0,1)$

Output: $\bar{\mathbf{x}}_{0:T}^{1:N}$ (N points in $\mathcal{X}^{T+1}$)

Find permutation τ such that $\bar{u}_T^{\tau(1)} \leq ... \leq \bar{u}_T^{\tau(N)}$

Compute $\bar{a}_T^n = F_{T,N}^{-1}(\bar{u}_T^{\tau(n)})$ where $F_{t,N}(m) = \sum_{i=1}^N W_T^{\sigma_T(i)} \mathbb{I}(i \leq m)$

Set $\bar{\mathbf{x}}_T^n = \mathbf{x}_T^{\bar{a}_T^n}$ and $\widetilde{W}_{T|T}^n = W_T^n$.

for $t = T-1 \to 0$ **do**

Find permutation τ such that $\bar{u}_t^{\tau(1)} \leq ... \leq \bar{u}_t^{\tau(N)}$

Set $\bar{\mathbf{x}}_t^n = \mathbf{x}_t^{\bar{a}_t^n}$ where $\bar{a}_t^n = \bar{F}_{t,N}^{-1}(\bar{u}_t^{\tau(n)})$ with $\bar{F}_{t,N}(m) = \sum_{i=1}^N \widetilde{W}_{t|T}^{\sigma_t(i)} \mathbb{I}(i \leq m)$,

$$\widetilde{W}_{t|T}^i = \sum_{j=1}^N \widetilde{W}_{t+1|T}^j \frac{\widetilde{W}_t^i(\mathbf{x}_{t+1}^j)}{\sum_{k=1}^N \widetilde{W}_t^k(\mathbf{x}_{t+1}^j)}, \quad i \in 1:N$$

and where $\widetilde{W}_t^i$ is defined by (2.34)

end for

$t^* \in 1:(T-1)$,

$$\widetilde{\mathbb{Q}}_T(\mathrm{d}\mathbf{x}_{0:T}) = \widetilde{\mathbb{Q}}_{t^*|T}(\mathrm{d}\mathbf{x}_{t^*}) \prod_{t=1}^{t^*} \mathcal{M}_{t,\mathbb{Q}_{t-1}}(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t-1}) \prod_{t=t^*+1}^{T} \widetilde{\mathcal{M}}_{t-1,\mathcal{P}_t}(\mathbf{x}_{t-1}, \mathrm{d}\mathbf{x}_t) \tag{2.37}$$

where, for any $\pi \in \mathcal{P}([0,1)^d)$, $\widetilde{\mathcal{M}}_{t-1,\pi} : [0,1)^d \to \mathcal{P}([0,1)^d)$ is a Markov kernel such that

$$\widetilde{\mathcal{M}}_{t-1,\pi}(\mathbf{x}_{t-1}, \mathrm{d}\mathbf{x}_t) = \frac{\widetilde{m}_{t-1}(\mathbf{x}_t, \mathbf{x}_{t-1})\pi(\mathrm{d}\mathbf{x}_t)}{\pi(\widetilde{m}_{t-1})(\mathbf{x}_{t-1})}, \quad \widetilde{m}_{t-1}(\mathbf{x}_t, \mathbf{x}_{t-1}) = \frac{\gamma_{t-1}(\mathbf{x}_{t-1}) m_t(\mathbf{x}_{t-1}, \mathbf{x}_t)}{\gamma_t(\mathbf{x}_t)}$$

with $(\gamma_t)_{t \geq 0}$ a user defined sequence of densities on $[0,1)^d$ and, for $t \in t^* : T$, $\mathcal{P}_t(\mathrm{d}\mathbf{x}_t)$ the marginal distribution of $\mathbf{x}_t$ relative to (using the convention that empty products equal to one)

$$\tilde{\mathcal{P}}_T(\mathrm{d}\mathbf{x}_{t^*:T}) = \frac{1}{\tilde{Z}_{\mathcal{P}}} \gamma_T(\mathrm{d}\mathbf{x}_T) G_T(\mathbf{x}_T) \prod_{t=t^*}^{T-1} G_t(\mathbf{x}_t) \tilde{m}_t(\mathbf{x}_{t+1}, \mathrm{d}\mathbf{x}_t). \tag{2.38}$$

In the sequel, $\tilde{Z}_{\mathcal{P}}$ is a normalizing constant and, to simplify the presentation, it is assumed that for all t the weight function G_t depends only on the current state $\mathbf{x}_t$.

For further simplification, assume that $\tilde{m}_{t-1}(\mathbf{x}_t, \mathbf{x}_{t-1})\mathrm{d}\mathbf{x}_{t-1}$ is a probability distribution. Then, the formulation (2.38) shows that $\mathcal{P}_t(\mathrm{d}\mathbf{x}_t)$ corresponds to the filtering

distribution at time t in the Feynman-Kac model $\{\tilde{m}_{T-t}, G_{T-t}\}_{t=0}^{T-t^*}$ with initial distribution $\tilde{m}_T(\mathrm{d}\mathbf{x}_0) = \gamma_T(\mathrm{d}\mathbf{x}_0)$. Therefore, a QMC version of the two filter SQMC smoothing algorithm is as follows:

Algorithm 2.4 SQMC two filter smoothing algorithm

1: Run the SQMC Algorithm 2.1 for the Feynman-Kac model $(m_t, G_t)_{t=0}^T$ to get an estimates $\widehat{\mathbb{Q}}_t^N$ of $\mathbb{Q}_t$ for $t \in 0:T$;

2: Run the SQMC Algorithm 2.1 for the Feynman-Kac model $(\tilde{m}_{T-t}, G_{T-t})_{t=0}^{T-t^*}$ to get an estimates $\widehat{\mathcal{P}}_t^N$ of $\mathcal{P}_t$ for $t \in (t^*+1):T$.

3: Run the backward Algorithm 2.3 up to time t^* to get an estimate $\widetilde{\mathbb{Q}}_{t^*|T}^N$ of $\widetilde{\mathbb{Q}}_{t^*|T}$.

4: Let $\tilde{\mathbf{u}}^{1:N}$ be a point set in $[0,1)^{T+1}$ and compute $h_{0:T}^{\mathrm{2F},n} = F^{-1}_{\widetilde{\mathbb{Q}}^{\mathrm{2F}}_{T,h_T}}(\tilde{\mathbf{u}}^n)$, $n \in 1:N$, with $\widetilde{\mathbb{Q}}^{\mathrm{2F}}_{T,h_T}$ the image by h_T of

$$\widetilde{\mathbb{Q}}_T^{\mathrm{2F}}(\mathrm{d}\mathbf{x}_{0:T}) = \widetilde{\mathbb{Q}}_{t^*|T}^N(\mathrm{d}\mathbf{x}_{t^*}) \prod_{t=1}^{t^*-1} \mathcal{M}_{t,\widehat{\mathbb{Q}}_t^N}(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t-1}) \prod_{t=t^*+1}^{T} \widetilde{\mathcal{M}}_{t-1,\widehat{\mathcal{P}}_t^N}(\mathbf{x}_{t-1}, \mathrm{d}\mathbf{x}_t).$$

5: For $n \in 1:N$, compute $\mathbf{x}_{0:T}^{\mathrm{2F},n} = H_T(h_{0:T}^{\mathrm{2F},n})$.

Theorem 2.1 provides conditions under which the estimates $\widehat{\mathbb{Q}}_t^N$ and $\widehat{\mathcal{P}}_t^N$ are consistent in the sense of the extreme metric. Corollary 2.2 shows that, under suitable assumptions on $(m_t, G_t)_{t\geq 0}$, Algorithm 2.3 gives an estimate $\widetilde{\mathbb{Q}}_{t^*|T}^N$ that is consistent for the marginal smoothing distribution $\widetilde{\mathbb{Q}}_{t^*|T}$ and therefore $\widetilde{\mathbb{Q}}_T^{\mathrm{2F}}$ is a convergent estimate of $\widetilde{\mathbb{Q}}_T$ if the Feynman-Kac models described in steps 1 and 2 verify the assumptions of Theorem 2.1. Finally, conditions for the validity of the steps 4-5 are given in Corollary 2.1 (note however that in the expression of $\widetilde{\mathbb{Q}}_T^{\mathrm{2F}}$ two Markov kernels depend on $\mathbf{x}_{t^*}$ but it is trivial to modify the proof of Corollary 2.1 to take this fact into account).

2.6 Numerical study

As in Gerber and Chopin (2014), we consider the following multivariate stochastic volatility model (SV) proposed by Chan et al. (2006):

$$\begin{cases} \mathbf{y}_t = S_t^{1/2}\boldsymbol{\epsilon}_t, & t \geq 0 \\ \mathbf{x}_t = \boldsymbol{\mu} + \Phi(\mathbf{x}_{t-1} - \boldsymbol{\mu}) + \Psi^{\frac{1}{2}}\boldsymbol{\nu}_t, & t \geq 1 \end{cases} \tag{2.39}$$

where $S_t = \mathrm{diag}(\exp(x_{t1}), ..., \exp(x_{td}))$, Φ and Ψ are diagonal matrices and $(\boldsymbol{\epsilon}_t, \boldsymbol{\nu}_t) \sim \mathcal{N}_{2d}(\mathbf{0}_{2d}, C)$ with C a correlation matrix.

The parameters we use for the simulations are the same as in Chan et al. (2006) in absence of leverage effect: $\phi_{ii} = 0.9$, $\mu_i = -9$, $\psi_{ii}^2 = 0.1$ for all $i = 1, ..., d$ and

$$C = \begin{pmatrix} 0.6\mathbf{1}_d + 0.4\mathcal{I}_d & \mathbf{0}_d \\ \mathbf{0}_d & 0.8\mathbf{1}_d + 0.2\mathcal{I}_d \end{pmatrix}$$

where $\mathcal{I}_d$ is the d-dimensional identity matrix, and $\mathbf{1}_d$ (respectively $\mathbf{0}_d$) is the $d \times d$ matrix having one (resp. zero) in all its entries. The prior distribution for $\mathbf{x}_0$ is the stationary distribution of the process $(\mathbf{x}_t)_{t \geq 0}$, which is also our choice for the distributions $\gamma_t(\mathrm{d}\mathbf{x}_t)$, $t \in 0 : T$. The simulations are done for $d = 2$ and $T = 399$ (i.e. 400 observations).

In this numerical study, we report results for the QMC backward pass (Algorithms 2.2), for the QMC backward pass which estimates the marginal smoothing distributions (Algorithm 2.3) and for QMC two filter smoothing (Algorithm 2.4 where, in step 3., Algorithm 2.3 is used). These algorithms are compared with their Monte Carlo counterpart using the gain factors for the estimation of the smoothing expectation $\mathbb{E}[x_{1t}|\mathbf{y}_{0:T}]$, $t \in 0 : T$, which we define as the Monte Carlo mean square error (MSE) over the quasi-Monte Carlo MSE. Results for the second component of $\mathbf{x}_t$ are not reported because, since the model is symmetric, they are similar to those for x_{1t}.

The implementation of QMC and Monte Carlo algorithms are as in Gerber and Chopin (2014). The QMC algorithms are based on Owen (1995) nested scrambled Sobol' sequence using the C++ library of T. Kollig and A. Keller (`http://www.uni-kl.de/AG-Heinrich/SamplePack.html`) while to sort the particles according to their Hilbert index we use the C++ library of Chris Hamilton (`http://web.cs.dal.ca/~chamilto/hilbert/index.html`). Prior to this sort step, the particles are mapped into $[0, 1)^d$ using a component-wise (rescaled) logistic transform.

The SMC algorithm and the Monte Carlo version of Algorithm 2.3 are implemented using systematic resampling (Carpenter et al., 1999) and, in all Monte Carlo algorithms, the random variables are generated using standard methods (i.e. not using the inverse Rosenblatt transformation). The complete C/C++ code is available on-line at `https://bitbucket.org/mgerber/sqmc`.

The first column of Figure 2.1 shows the results for the three smoothing algorithms when $N = 2^8$ particles are used. Looking first at the results for Algorithm 2.2 (plots on the first line of Figure 2.1), we see that the MSE of the QMC algorithm is in all cases smaller than for its Monte Carlo counterpart, except in one time step. The gain factor is larger than 2 for 280 values of t and is larger than three for 23% of the time steps. Note that because the algorithms have complexity $\mathcal{O}(N^2)$ (and have very similar running times in our implementation) these gains of QMC smoothing for a fixed number of particles translate to important savings in term of running time if one want to reach a given approximation error.

The graphs in the middle of Figure 2.1 present the results for the marginal smoothing algorithm (Algorithm 2.3). As can be observed, the gain factors are

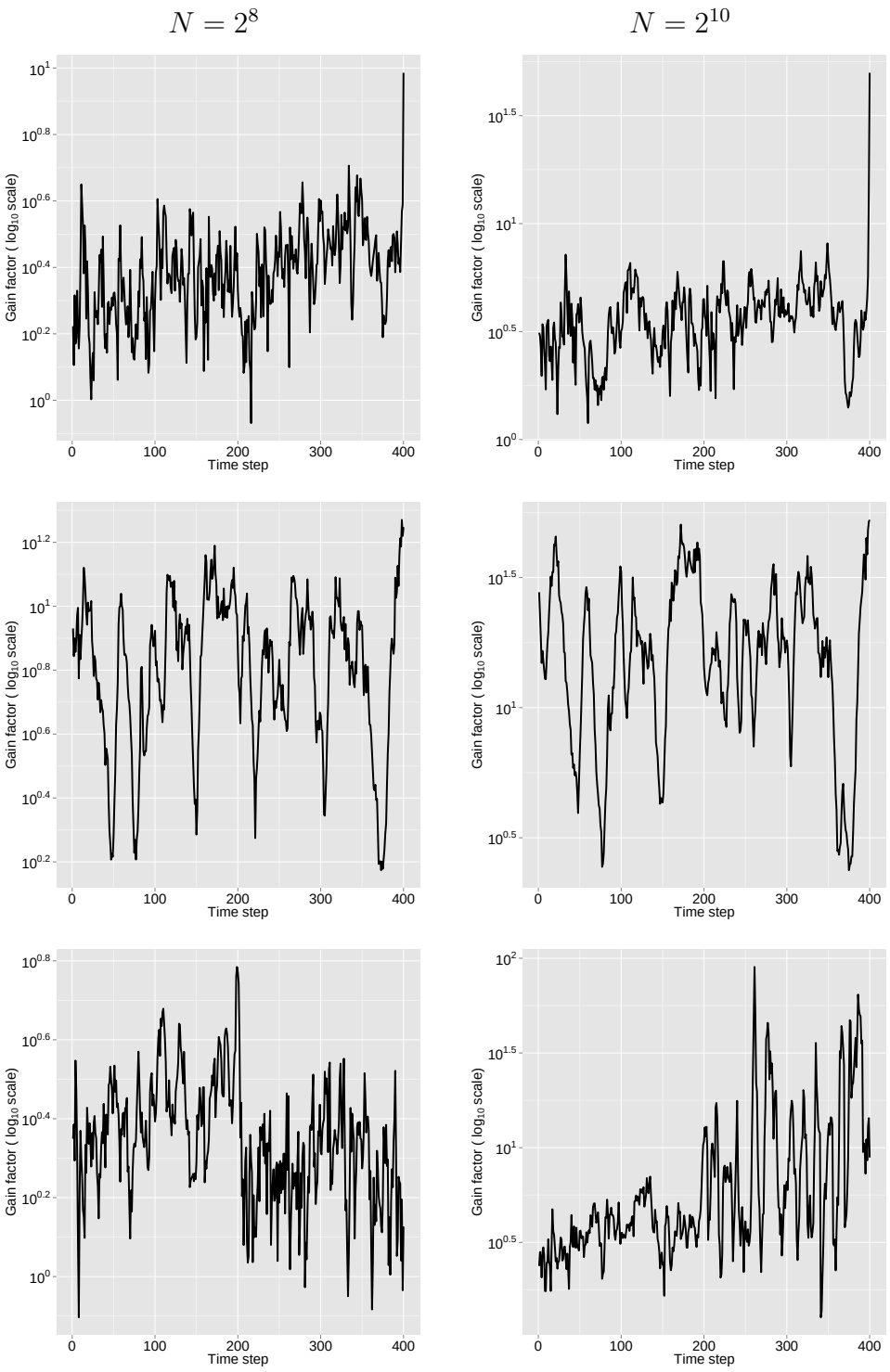

Figure 2.1: Smoothing of the bivariate SV model (2.39) with $N = 2^8$ and $N = 2^8$ particles. The graphs give the ratio of the SMC and SQMC MSEs for the estimation of $\mathbb{E}[x_{t1}|\mathbf{y}_{0:T}]$ as a function of t, and are obtained from 100 replications. The first line gives the result for Algorithm 2.2, the second line for Algorithm 2.3 and the last line for Algorithm 2.4.

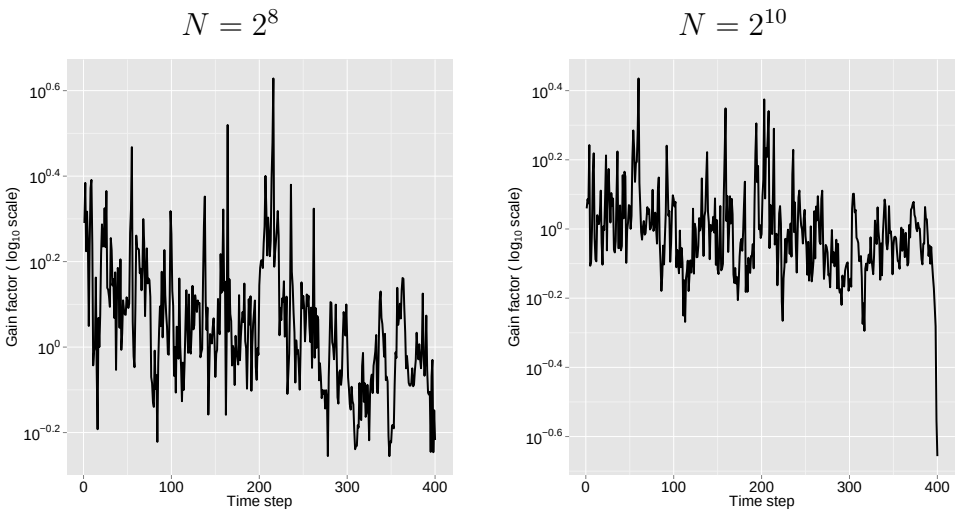

Figure 2.2: Smoothing of the bivariate SV model (2.39). The graphs give the ratio of the hybrid forward-backward smoothing and the plain QMC forward-backward smoothing MSEs for the estimation of $\mathbb{E}[x_{t1}|\mathbf{y}_{0:T}]$ as a function of t, and are obtained from 100 replications.

higher than for Algorithm 2.2 (and in all cases greater than 1), with reductions of MSEs by factors between $10^{0.5}$ and 10 for the vast majority of the 400 time steps. Because the algorithms have complexity $\mathcal{O}(N^2)$, a gain of 10 for QMC smoothing means that we should multiply the running time of its Monte Carlo counterpart by 100 in order to reach the same MSE (assuming that we are in the asymptotic regime where the Monte Carlo MSE deceases linearly with N). The gain factors for Algorithm 2.3 are higher than for Algorithm 2.2 because the former is based on QMC point sets of dimension 1 while the latter is based on a QMC point set of dimension 400, which exhibits poor equidistribution properties, as explained in Section 2.4.4. The last graphs in Figure 2.1 show the results for two filter smoothing (Algorithm 2.4) with $t^* = 200$. The high gain factor obtained at time $t = t^*$ arises because we estimate $\widetilde{\mathbb{Q}}_{t^*|T}$ using Algorithm 2.3 which, as we have just seen, is much more efficient than its Monte Carlo counterpart. For $t \in 0 : t^*$, we note that the gain factors are globally higher to what was obtained with the Algorithm 2.2 while, for $t > t^*$ they are globally smaller.

The second column of Figure 2.1 presents the results for $N = 2^{10}$. Compared to the graphs shown in the first column of the same figure, we observe that the gain factors are globally higher, showing that the gain of QMC smoothing over plain Monte Carlo smoothing increases with the number of particles. The gain factors for Algorithm 2.2 are around $10^{0.5}$ in average while, for Algorithm 2.3, they are larger than 10 for 304 time steps. Interestingly, for these two algorithms, no trend is observed in the evolution of the gain factors. Concerning the results for two filter

smoothing, we see an important difference between the gain for $t < t^*$ with those for $t \geq t^*$. While, in the first case, they are logically similar to those obtained with Algorithm 2.2, they are much higher when $t \geq t^*$, with values larger than 10 in 97 of the remaining 200 time steps. Combined with the results obtained for $N = 2^8$ particles, this suggests that the gain of QMC filtering/smoothing methods for the Feynman-Kac model $\{\tilde{m}_{T-t}, G_{T-t}\}_{t=0}^{T-t^*}$ increases faster than for the original model.

Finally, Figure 2.2 compares plain QMC forward-backward smoothing with the hybrid strategy which consists to use SQMC (Algorithm 2.1) combined with a standard Monte Carlo backward pass. Results are reported in Figure 2.2 both for $N = 2^8$ and for $N = 2^{10}$. As one can observed, plain QMC forward-backward smoothing becomes relatively less efficient as $T - t$ increases and is dominated by the hybrid strategy for $T - t$ large enough. From the discussion of Section 2.4.4, this result is quite intuitive. Indeed, as $T - t$ increases, the dimension of the QMC point set used in the backward step increases as well and hence its equidistribution properties deteriorate. The graphs presented in Figure 2.2 therefore suggests that the optimal strategy consist to use as input for the backward pass of SQMC a point set $\tilde{\mathbf{u}}^{1:N}$ in $[0,1)^{T+1}$, $\tilde{\mathbf{u}}^n = (\tilde{\mathbf{u}}_1^n, \tilde{\mathbf{u}}_2^n)$, such that for a $\tilde{T} \in 1 : (T-1)$, $\tilde{\mathbf{u}}_1^{1:N}$ is a QMC point set in $[0,1)^{\tilde{T}}$ and $\tilde{\mathbf{u}}_2^{1:N}$ is a set of independent uniform random variates in $[0,1)^{T+1-\tilde{T}}$. Note that the point set $\tilde{\mathbf{u}}^{1:N}$ is such that, as $N \to +\infty$, $D(\tilde{\mathbf{u}}^{1:N}) \to 0$ almost surely (Ökten et al., 2006, Theorem 5) and therefore it satisfies the conditions of Theorem 2.3.

2.7 Conclusion

On the one hand, the estimation of the smoothing distribution $p(\mathbf{x}_{0:T}|\mathbf{y}_{0:T})$ is a challenging task for QMC methods because it is typically a high dimensional problem. On the other hand, due to the $\mathcal{O}(N^2)$ complexity of most smoothing algorithms, small gains in term of mean square errors translate into important savings in term of running times to reach the same level of error. In this work we provide asymptotic results for some QMC smoothing strategies, namely forward smoothing, forward-backward smoothing and two filter smoothing. In a simulation study we show that the QMC forward-backward smoothing algorithm outperforms its Monte Carlo counterpart despite of the high dimensional nature of the problem. Also, if one is interested in the estimation of the marginal smoothing distributions, much more important gains can be obtained because we can derive a backward step which rely only on univariate QMC point sets.

The set of smoothing strategies discussed in this work is obviously not exhaustive. For instance, Fearnhead et al. (2010) proposed a smoothing algorithm that only costs $\mathcal{O}(N)$ operations. Although not discussed in this paper, our analysis can be trivially applied to derive a QMC version of this algorithm and to provide conditions for its validity. An other interesting smoothing algorithm is proposed in Douc et al. (2011),

where the backward pass is an accept-reject procedure. Compared to standard forward-backward smoothing, this alternative backward pass only requires $\mathcal{O}(N)$ operations and therefore reaches the same complexity as the method proposed in Fearnhead et al. (2010). A last interesting smoothing strategy is the particle Gibbs sampler proposed by Andrieu et al. (2010) which generates a Markov chain having the smoothing distribution as stationary distribution. For these last two methods, the usefulness and the validity of replacing pseudo-random numbers by QMC point sets remain interesting open questions.

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Appendix: Proofs

A Main properties of the Hilbert curve

The proofs of the results presented in this work are based on the following technical properties of H and H_m. For $m \geq 0$, let $\mathcal{I}_m^d = \left\{I_m^d(k)\right\}_{k=0}^{2^{md}-1}$ be the collection of consecutive closed intervals in $[0,1]$ of equal size 2^{-md} and such that $\cup\mathcal{I}_m^d = [0,1]$. For $k \geq 0$, $S_m^d(k) = H_m(I_m^d(k))$ belongs to $\mathcal{S}_m^d$, the set of the 2^{md} closed hypercubes of volume 2^{-md} that covers $[0,1]^d$, $\cup\mathcal{S}_m^d = [0,1]^d$; $S_m^d(k)$ and $S_m^d(k+1)$ are adjacent, i.e. have at least one edge in common (*adjacency property*). If we split $I_m^d(k)$ into the 2^d successive closed intervals $I_{m+1}^d(k_i)$, $k_i = 2^d k + i$ and $i \in 0 : 2^d - 1$, then the $S_{m+1}^d(k_i)$'s are simply the splitting of $S_m^d(k)$ into 2^d closed hypercubes of volume $2^{-d(m+1)}$ (*nesting property*). Finally, the limit H of H_m has the *bi-measure property*: $\lambda_1(A) = \lambda_d(H(A))$, for any measurable set $A \subset [0,1]$, and satisfies the *Hölder condition* $\|H(x_1) - H(x_2)\| \leq C_H |x_1 - x_2|^{1/d}$ for all x_1 and x_2 in $[0,1]$.

B Preliminary results: Proofs of Section 2.2

B.1 Proof of Theorem 2.2

The prove of this result is an adaptation of the the proof of Hlawka and Mück (1972, "Satz 2").

In what follows, we use the shorthand $\alpha_N(B) = \mathcal{S}(\mathbf{u}^{1:N})(B)$ for any set $B \subset [0,1)^d$. One has

$$\|\mathcal{S}(\mathbf{x}^{1:N}) - \pi\|_{\mathrm{E}} = \sup_{B \in \mathcal{B}_{[0,1)^d}} \left|\alpha_N\left(F_\pi(B)\right) - \lambda_d\left(F_\pi(B)\right)\right|$$

Let $\beta = \lceil \kappa^{-1} \rceil$, $\tilde{d} = \sum_{i=0}^{d-1} \beta^i$ and $\mathcal{P}$ be the partition of $[0,1)^d$ in $L^{\tilde{d}}$ congruent hyperrectangles W of size $L^{-\beta^{d-1}} \times ... \times L^{-1}$. Let $B \in \mathcal{B}_{[0,1)^d}$, $\mathcal{U}_1$ the set of the elements of $\mathcal{P}$ that are strictly in $F_\pi(B)$, $\mathcal{U}_2$ the set of elements $W \in \mathcal{P}$ such that $W \cap \partial(F_\pi(B)) \neq \varnothing$, $U_1 = \cup\,\mathcal{U}_1$, $U_2 = \cup\,\mathcal{U}_2$, and $U_1' = F_\pi(B) \setminus U_1$ so that (Hlawka and Mück, 1972, "Satz 2" or Gerber and Chopin, 2014, Theorem 4)

$$\left|\alpha_N\left(F_\pi(B)\right) - \lambda_d\left(F_\pi(B)\right)\right| \leq \left|\alpha_N(U_1) - \lambda_d(U_1)\right| + \#\mathcal{U}_2 \left\{D(\mathbf{u}^{1:N}) + L^{-\tilde{d}}\right\}$$

where, under the assumption of the theorem, $|\alpha_N(U_1) - \lambda_d(U_1)| \leq L^{\tilde{d}-1} D(\mathbf{u}^{1:N})$ (see Hlawka and Mück, 1972).

To bound $\#\mathcal{U}$, let $\mathcal{P}'$ be the partition of $[0,1)^d$ into hyperrectangles W' of size $L'^{-\beta^{d-1}} \times ... \times L'^{-1}$ such that, for all points $\mathbf{x}$ and $\mathbf{x}'$ in W', we have

$$|F_i(x_{1:i-1}, x_i) - F_i(x'_{1:i-1}, x'_i)| \leq L^{-\beta^{d-i}}, \quad i = 1, ..., d \tag{2.40}$$

where $F_i(x_{1:i-1}, x_i)$ denotes the i-th component of $F_\pi(\mathbf{x})$ (with $F_i(x_{1:i-1}, x_i) = F_1(x_1)$ when $i = 1$). To that effect, let $i \in 2:d$ and note that

$$\begin{aligned}|F_i(x_{1:i-1}, x_i) - F_i(x'_{1:i-1}, x'_i)| \leq |F_i(x_{1:i-1}, x_i) - F_i(x_{1:i-1}, x'_i)| \\ + |F_i(x_{1:i-1}, x'_i) - F_i(x'_{1:i-1}, x'_i)|.\end{aligned}$$

By Assumption 3, the probability measure $\pi_i(x_{1:i-1}, \mathrm{d}x_i)$ admits a density $p_i(x_i|x_{1:i-1})$ with respect to the Lebesgue measure such that $\|p_i(\cdot|\cdot)\|_\infty < +\infty$. Therefore, the first term after the inequality sign is bounded by $\|p_i\|_\infty L'^{-\beta^{d-i}}$. For the second term, the Hölder property of F_π implies that

$$|F_i(x_{1:i-1}, x'_i) - F_i(x'_{1:i-1}, x'_i)| \leq C_\pi (L'^{-\beta^{d+1-i}})^\kappa \leq C_\pi (L'^{-\beta^{d+1-i}})^{1/\beta} = C_\pi L'^{-\beta^{d-i}}$$

with C_π the Hölder constant of F_π. For $i = 1$, we simply have

$$|F_1(x_1) - F_1(x'_1)| \leq \|p_1\|_\infty L'^{-\beta^{d-1}}.$$

Condition (2.40) is therefore verified for L' the smallest integer such that $L' \geq \tilde{C}L$, where

$$\tilde{C} = \max\{(\|p_i\|_\infty + C_\pi)^{-\beta^{d-i}}, i \in 1:d\}.$$

Remark now that $\partial(F_\pi(B)) = F_\pi(\partial(B))$ since F is a continuous function. Let $R \in \partial B$ be a $(d-1)$-dimensional face of B and $\mathcal{R}$ be the set of hyperrectangles $W' \in \mathcal{P}'$ such that $R \cap W' \neq \varnothing$. Note that $\#\mathcal{R} \leq L'^{\tilde{d}-1} \leq (\lfloor \tilde{C}L \rfloor + 1)^{\tilde{d}-1}$. For each $W' \in \mathcal{R}$, take a point $\mathbf{r}^{W'} \in R \cap W'$ and define

$$\tilde{\mathbf{r}}^{W'} = F_\pi(\mathbf{r}^{W'}) \in F_\pi(R).$$

Let $\tilde{\mathcal{R}}$ be the collection of hyperrectangles $\tilde{W}$ of size $2L^{-\beta^{d-1}} \times ... \times 2L^{-1}$ and having point $\tilde{\mathbf{r}}^{W'}$, $W' \in \mathcal{R}$, as middle point.

For an arbitrary $\mathbf{u} \in F_\pi(R)$, let $\mathbf{x} = F_\pi^{-1}(\mathbf{u}) \in R$. Hence, $\mathbf{x}$ is in one hyperrectangle $W' \in \mathcal{R}$ so that using (2.40)

$$|u_i - \tilde{r}_i^{W'}| = |F_i(x_{1:i-1}, x_i) - F_i(r_{1:i-1}^{W'}, r_i^{W'})| \leq L^{-\beta^{d-i}}, \quad i = 1, \ldots, d.$$

This shows that $\mathbf{u}$ belongs to the hyperrectangle $\tilde{W} \in \tilde{\mathcal{R}}$ with center $\tilde{\mathbf{r}}^{W'}$ so that $F_\pi(R)$ is covered by at most $\#\tilde{\mathcal{R}} = \#\mathcal{R} \leq (\lfloor \tilde{C}L \rfloor + 1)^{\tilde{d}-1}$ hyperrectangles $\tilde{W} \in \tilde{\mathcal{R}}$.

To go back to the initial partition of $[0,1)^d$ with hyperrectangles in $\mathcal{P}$, remark that every hyperrectangles in $\tilde{\mathcal{R}}$ is covered by at most c_1^* hyperrectangles in $\mathcal{P}$ for a constant c_1^*. Finally, since the set ∂B is made of the union of $2d$ $(d-1)$-dimensional faces of B, we have $\#\mathcal{U}_2 \leq c_2^* L^{\tilde{d}-1}$ for a constant c_2^*.

Then, we may conclude the proof as follows

$$\|\mathcal{S}(\mathbf{x}^{1:N}) - \pi\|_{\mathrm{E}} \leq L^{\tilde{d}-1} D(\mathbf{u}^{1:N}) + c_2^* L^{\tilde{d}-1} \left(D(\mathbf{u}^{1:N}) + L^{-\tilde{d}} \right)$$

where the optimal value of L is such that

$$\|\mathcal{S}(\mathbf{x}^{1:N}) - \pi\|_{\mathrm{E}} \leq c_3^* D(\mathbf{u}^{1:N})^{1/\tilde{d}}$$

for a constant c_3^*

B.2 Proof of Theorem 2.3

Let $m \geq 0$ be an arbitrary integer, $B \in \mathcal{B}_{[0,1)^d}$ be such that $S_m^d(k) \subseteq B$ for at least one $k \in \{0, \ldots, 2^{dm}-1\}$ and $k_{m,B}$ be the smallest of these k's. Let $\mathcal{S}_m^B = \{W \in \mathcal{S}_m^d : W \subseteq B\}$, $\tilde{B} = \cup \tilde{\mathcal{S}}_m^B$ and $\mathcal{D}_m^B = \{W \in \mathcal{S}_m^d : (B \setminus \tilde{B}) \cap W \neq \varnothing\}$. Let $\tilde{\mathcal{D}}_m^B$ the set of $\#\mathcal{D}_m^B$ disjoint subsets of $[0,1)^d$ such that (i) $\forall \tilde{W} \in \tilde{\mathcal{D}}_m^B$, there exists a $W \in \mathcal{D}_m^B$ such that $\tilde{W} \subseteq W$, (ii) $\cup \tilde{\mathcal{D}}_m^B = \mathcal{D}_m^B$ and (iii) $\tilde{B} \cap \{\cup \tilde{\mathcal{D}}_m^B\} = \varnothing$; that is, $\tilde{\mathcal{D}}_m^B$ is obtained by removing boundaries of the elements in $\mathcal{D}_m^B$ such that conditions (ii) and (iii) are verified.

Then,

$$\left|\pi^N(B) - \pi(B)\right| \leq \left|\pi^N(\tilde{B}) - \pi(\tilde{B})\right| + \sum_{\tilde{W} \in \tilde{\mathcal{D}}_m^B} \left|\pi^N(\tilde{W} \cap B) - \pi(\tilde{W} \cap B)\right|. \quad (2.41)$$

To bound the first term on the right-hand side, let

$$\tilde{\mathcal{S}}_m^B = \{S_m^d(k_{m,B})\} \cup \{S_m^d(k) \in \mathcal{S}_m^d,\, k > k_{m,B} : S_m^d(k) \subseteq B, S_m^d(k-1) \cap B^c \neq \varnothing\}.$$

so that $\tilde{B}$ contains $\#\tilde{\mathcal{S}}_m^B$ non-consecutive hypercubes belonging to $\mathcal{S}_m^d$. By the property of the Hilbert curve, consecutive hypercubes in $\mathcal{S}_m^d$ correspond to consecutive intervals in $\mathcal{I}_m^d$ (adjacency property). Therefore, $h(\tilde{B})$ contains at most $\#\tilde{\mathcal{S}}_m^B$ non consecutive intervals that belongs to $\mathcal{I}_m^d$ so that there exists disjoint closed intervals $I_j \subset [0,1)$, $j = 1, ..., \#\tilde{\mathcal{S}}_m^B + 1$, such that $h(\tilde{B}) = \cup_{j=1}^{\#\tilde{\mathcal{S}}_m^B + 1} I_j$. Hence,

$$\left|\pi^N(\tilde{B}) - \pi(\tilde{B})\right| = \left|\pi_h^N(h(\tilde{B})) - \pi_h(h(\tilde{B}))\right| \leq (\#\tilde{\mathcal{S}}_m^B + 1) r(N)$$

where $r(N) = \|\pi_h^N - \pi_h\|_{\mathrm{E}}$.

To bound $\tilde{\mathcal{S}}_m^B$, let $m_1 \leq m$ be the smallest positive integer such that $S_{m_1}^d(k) \subseteq B$ for at least one $k \in \{0, \ldots, 2^{dm_1} - 1\}$ and let $k_{m_1}^*$ be the maximal number of

hypercubes in $\mathcal{S}^B_{m_1}$. Note that $k^*_{m_1} = 2^{m_1(d-1)}$. Indeed, by the definition of m_1, the only way for B to be made of more than one hypercube in $\mathcal{S}^d_{m_1}$ is to stack such hypercubes in at most $(d-1)$ dimension (otherwise we can reduce m_1 to $m_1 - 1$ by the nesting property of the Hilbert curve and because B is a hyperrectangle) and in each dimension we can stack at most 2^{m_1} hypercubes that belong to $\mathcal{S}^B_{m_1}$. Let $m_2 = m_1 + 1$ and $B_{m_2} = B \setminus \cup\mathcal{S}^B_{m_1}$. Then, $\#\mathcal{S}^{B_{m_2}}_{m_2} \leq k^*_{m_2} := 2d2^{m_2(d-1)}$. Indeed, by construction, $\#\mathcal{S}^{B_{m_2}}_{m_2}$ is the number of hypercubes in $\mathcal{S}^d_{m_2}$ required to cover the faces of the hyperrectangle made by the union of the hypercubes in $\mathcal{S}^B_{m_1}$. This hyperrectangle has at most $2d$ faces of dimension $(d-1)$. The volume of each face is smaller than one so that we need at most $2^{m_2(d-1)}$ hypercubes in $\mathcal{S}^d_{m_2}$ to cover each faces.

More generally, for $m_1 \leq m_k \leq m$, we define $B_{m_k} = B_{m_{k-1}} \setminus \cup\mathcal{S}^{B_{m_{k-1}}}_{m_k-1}$ and $\#\mathcal{S}^{B_{m_k}}_{m_k}$ is bounded $k^*_{m_k} := 2d2^{m_k(d-1)}$ (simply note that, for any $j = 1, ..., k-1$, the union of all hypercubes belonging to $\mathcal{S}^{B_{m_j}}_{m_j}$ form a hyperrectangles having at most $2d$ faces of dimension $(d-1)$). Therefore, since $d \geq 2$,

$$\#\tilde{\mathcal{S}}^B_m \leq k^*_m + \sum_{j=m_1}^{m-1} k^*_j = 2d2^{m(d-1)} + 2d2^{m_1(d-1)} \frac{2^{(m-m_1)(d-1)} - 1}{2^{d-1} - 1} \leq (4d)\, 2^{m(d-1)}$$

so that

$$\left|\pi^N(\tilde{B}) - \pi(\tilde{B})\right| \leq [1 + (4d)2^{m(d-1)}]r(N).$$

For the second term of (2.41), take $\tilde{W} \in \tilde{\mathcal{D}}^B_m$, and note that $\tilde{W} \subseteq S^d_m(k)$ for a $k \in \{0, \ldots, 2^{dm} - 1$. Then,

$$\begin{aligned}\left|\pi^N(\tilde{W} \cap B) - \pi(\tilde{W} \cap B)\right| &\leq \pi^N(S^d_m(k)) + \pi(S^d_m(k)) \\ &\leq 2\pi(S^d_m(k)) + r(N) \\ &= 2\|\pi\|_\infty 2^{-dm} + r(N).\end{aligned}$$

Thus,

$$\sum_{\tilde{W} \in \tilde{\mathcal{D}}^B_m} \left|\pi^N(\tilde{W} \cap B) - \pi(\tilde{W} \cap B)\right| \leq 4d\|\pi\|_\infty 2^{-m} + 2d2^{m(d-1)} r(N) \tag{2.42}$$

since $\#\tilde{\mathcal{D}}^B_m = \#\mathcal{D}^B_m \leq 2d2^{m(d-1)}$. Indeed, by construction, $\#\mathcal{D}^B_m$ is the number of hypercubes in $\mathcal{S}^d_m$ required to cover the faces of the hyperrectangle made by the union of the hypercubes in $\mathcal{S}^B_m$. This hyperrectangle has $2d$ faces of dimension $(d-1)$. The volume of each face is smaller than one so that we need at most $2d\, 2^{(d-1)m}$ hypercubes in $\mathcal{S}^d_m$ to cover each face.

Hence, for all $B \in \mathcal{B}_{[0,1)^d}$, such that $S^d_m(k) \subseteq B$ for a $k \in \{0, \ldots, 2^{dm} - 1\}$, we have

$$|\pi^N(B) - \pi(B)| \leq 4d\|\pi\|_\infty 2^{-m} + (1 + 6d2^{m(d-1)})r(N)$$

Finally, if $B \in \mathcal{B}_{[0,1)^d}$ is such that there exists no $k \in \{0, \dots, 2^{dm} - 1\}$ such that $S_m^d(k) \subseteq B$, we proceed exactly as above, but now $\tilde{B}$ is empty and therefore the first term in (2.41) disappears. To conclude the proof, note that the optimal value of m such that $2^{-m} \sim 2^{(d-1)m} r(N)$. Hence, $\|\pi^N - \pi\|_{\mathrm{E}} \leq c\, r(N)^{1/d}$ for a constant c.

B.3 Proof of Corollary 2.1

The proof of this corollary follows the lines of the proof of Theorem 2.3. Let $m \in \mathbb{N}$, $B' = B \times B_1$ where $B \in \mathcal{B}_{[0,1)^d}$ and $B_1 \in \mathcal{B}_{[0,1)^s}$. Then, using (2.41),

$$\begin{aligned}
\left|\mathcal{S}(P^N)(B') - \pi^N \otimes K(B')\right| &\leq \left|\mathcal{S}(P^N)(\tilde{B} \times B_1) - \pi^N \otimes K(\tilde{B} \times B_1)\right| \\
&\quad + \sum_{\tilde{W} \in \tilde{\mathcal{D}}_m^B} \left|\mathcal{S}(P^N)(\tilde{W} \cap B \times B_1) - \pi \otimes K(\tilde{W} \cap B \times B_1)\right| \\
&\leq \left|\mathcal{S}(P^N)(\tilde{B} \times B_1) - \pi^N \otimes K(\tilde{B} \times B_1)\right| \\
&\quad + \sum_{\tilde{W} \in \tilde{\mathcal{D}}_m^B} \left\{\mathcal{S}(P^N)(\tilde{W} \times [0,1)^s) + \pi(\tilde{W})\right\}
\end{aligned}$$

where each term after the last inequality sign can be bounded following exactly the same steps as in the proof of Theorem 2.3, with $r(N) = \|\mathcal{S}(P^N) - \pi^N \otimes K\|_{\mathrm{E}}$.

C Backward decomposition: Theorem 2.1

Lemma 10 of Gerber and Chopin (2014) is central for the proof of this result and is reproduced here for sake of completeness.

Lemma 2.1. *Let $(\pi^N \otimes K)_{N \geq 1}$ be a sequence of probability measures on $[0,1)^{d_1+d_2}$. Assume that $\|\pi^N - \pi\|_{\mathrm{E}} \to 0$ as $N \to +\infty$, for a $\pi \in \mathcal{P}([0,1)^{d_1})$, and that $F_K(\mathbf{x}_1, \mathbf{x}_2)$ is Hölder continuous with its i-th component strictly increasing in x_{2i}, $i \in 1 : d_2$. Then*

$$\|\pi^N \otimes K - \pi \otimes K\|_{\mathrm{E}} = o(1).$$

Let us now prove the theorem. The proof of (2.32) is a direct consequence of Gerber and Chopin (2014, Theorem 1). Indeed, let Ψ_t be the Bolzmann-Gibbs transformation associated to $G_t(H(h_{t-1}), \mathbf{x}_t)$ (see Del Moral, 2004, Definition 2.3.4). Then, for $\mathbf{x}_{t+1} \in [0,1)^d$, $t \geq 1$, note that $\mathcal{M}_{t+1,\mathbb{Q}_t}$ is the marginal of $\mathbf{x}_t$ relative to

$$\pi(\mathbf{x}_{t+1}, \mathrm{d}(\mathbf{x}_t, h_{t-1})) := \tilde{G}_{t+1}(\mathbf{x}_t, \mathbf{x}_{t+1}) \Psi_t(\mathbb{Q}_{t-1,h} \otimes m_{t,h})(\mathrm{d}(\mathbf{x}_t, h_{t-1}))$$

and that the Radon-Nikodym derivative

$$\frac{\pi(\mathbf{x}_{t+1}, \mathrm{d}(\mathbf{x}_t, h_{t-1}))}{\mathbb{Q}_{t-1,h} \otimes m_{t,h}(\mathrm{d}(\mathbf{x}_t, h_{t-1}))} \propto \tilde{G}_{t+1}(\mathbf{x}_t, \mathbf{x}_{t+1}) G_t(H(h_{t-1}), \mathbf{x}_t) \tag{2.43}$$

is continuous and bounded (by the assumption on $\tilde{G}_{t+1}$, by Assumption 1 of Theorem 2.1 and by the continuity of the Hilbert curve). By Theorem 2.1,

$$\|\mathcal{S}(h(\check{\mathbf{x}}_{t-1}^{1:N}), \mathbf{x}_t^{1:N}) - \mathbb{Q}_{t-1,h} \otimes m_{t,h}\|_{\mathrm{E}} = o(1)$$

and therefore Gerber and Chopin (2014, Theorem 1) implies, for $t \geq 1$,

$$\|\mathcal{M}_{t+1,\widehat{\mathbb{Q}}_t^N}(\mathbf{x}_{t+1}, \mathrm{d}\mathbf{x}_t) - \mathcal{M}_{t+1,\mathbb{Q}_t}(\mathbf{x}_{t+1}, \mathrm{d}\mathbf{x}_t)\|_{\mathrm{E}} = o(1), \quad \forall \mathbf{x}_{t+1} \in [0,1)^d.$$

To see that the $o(1)$ term in the above expression does not depend on $\mathbf{x}_{t+1}$ when $\|m_{t+1}\|_\infty < +\infty$, note that the proposal $\mathbb{Q}_{t-1} \otimes m_t$ does not depends $\mathbf{x}_{t+1}$, the Radon-Nikodym derivative (2.43) is bounded uniformly on $\mathbf{x}_{t+1}$ and therefore the results follows from the computations in the proof of Gerber and Chopin (2014, Theorem 1). This shows (2.32) for $t \geq 1$. To prove (2.32) for $t = 1$ replace $\mathbb{Q}_{t-1} \otimes m_t$ by m_0 in the above argument.

Let us now prove the second part of the theorem. As a preliminary result to establish (2.33) we show that, for all $t \geq 0$,

$$\|\widehat{\mathbb{Q}}_{t+1}^N \otimes \mathcal{M}_{t+1,\widehat{\mathbb{Q}}_t^N} - \mathbb{Q}_{t+1} \otimes \mathcal{M}_{t+1,\mathbb{Q}_t}\|_{\mathrm{E}} = o(1). \tag{2.44}$$

Let B_t and B_{t+1} be two sets in $\mathcal{B}_{[0,1)^d}$ and note $B_{t:t+1} = B_t \times B_{t+1}$ to simplify the notations. Then,

$$\begin{aligned}
&\left|\widehat{\mathbb{Q}}_{t+1}^N \otimes \mathcal{M}_{t+1,\widehat{\mathbb{Q}}_t^N}(B_{t:t+1}) - \mathbb{Q}_{t+1} \otimes \mathcal{M}_{t+1,\mathbb{Q}_t}(B_{t:t+1})\right| \\
&= \left|\int_{B_{t+1}} \lambda_d\left(F_{\mathcal{M}_{t+1,\widehat{\mathbb{Q}}_t^N}}(\mathbf{x}_{t+1}, B_t)\right) \widehat{\mathbb{Q}}_{t+1}^N(\mathrm{d}\mathbf{x}_{t+1}) - \lambda_d\left(F_{\mathcal{M}_{t+1,\mathbb{Q}_t}}(\mathbf{x}_{t+1}, B_t)\right) \mathbb{Q}_{t+1}(\mathrm{d}\mathbf{x}_{t+1})\right| \\
&\leq \left|\int_{B_{t+1}} \lambda_d\left(F_{\mathcal{M}_{t+1,\mathbb{Q}_t}}(\mathbf{x}_{t+1}, B_t)\right) \left(\widehat{\mathbb{Q}}_{t+1}^N - \mathbb{Q}_{t+1}\right)(\mathrm{d}\mathbf{x}_{t+1})\right| \\
&+ \left|\int_{B_{t+1}} \widehat{\mathbb{Q}}_{t+1}^N(\mathrm{d}\mathbf{x}_{t+1}) \left[\lambda_d\left(F_{\mathcal{M}_{t+1,\widehat{\mathbb{Q}}_t^N}}(\mathbf{x}_{t+1}, B_t)\right) - \lambda_d\left(F_{\mathcal{M}_{t+1,\mathbb{Q}_t}}(\mathbf{x}_{t+1}, B_t)\right)\right]\right|.
\end{aligned}$$

By assumption, $F_{\mathcal{M}_{t+1,\mathbb{Q}_t}}(\mathbf{x}_{t+1}, \mathbf{x}_t)$ is Hölder continuous. Since $\|\widehat{\mathbb{Q}}_{t+1}^N - \mathbb{Q}_{t+1}\|_{\mathrm{E}} = o(1)$ by Theorem 2.1, Lemma 2.1 therefore implies

$$\sup_{B_{t:t+1} \in \mathcal{B}^2_{[0,1)^d}} \left|\int_{B_{t+1}} \lambda_d\left(F_{\mathcal{M}_{t+1,\mathbb{Q}_t}}(\mathbf{x}_{t+1}, B_t)\right) \left(\widehat{\mathbb{Q}}_{t+1}^N - \mathbb{Q}_{t+1}\right)(\mathrm{d}\mathbf{x}_{t+1})\right| = o(1).$$

In addition,

$$\begin{aligned}
&\left|\int_{B_{t+1}} \widehat{\mathbb{Q}}_{t+1}^N(\mathrm{d}\mathbf{x}_{t+1}) \left[\lambda_d\left(F_{\mathcal{M}_{t+1,\widehat{\mathbb{Q}}_t^N}(\mathbf{x}_{t+1},B_t)}\right) - \lambda_d\left(F_{\mathcal{M}_{t+1,\mathbb{Q}_t}(\mathbf{x}_{t+1},B_t)}\right)\right]\right| \\
&\leq \int_{B_{t+1}} \widehat{\mathbb{Q}}_{t+1}^N(\mathrm{d}\mathbf{x}_{t+1}) \sup_{B_t\in\mathcal{B}_{[0,1)^d}} \left|\lambda_d\left(F_{\mathcal{M}_{t+1,\widehat{\mathbb{Q}}_t^N}(\mathbf{x}_{t+1},B_t)}\right) - \lambda_d\left(F_{\mathcal{M}_{t+1,\mathbb{Q}_t}(\mathbf{x}_{t+1},B_t)}\right)\right| \\
&\leq \int_{B_{t+1}} \widehat{\mathbb{Q}}_{t+1}^N(\mathrm{d}\mathbf{x}_{t+1}) \sup_{\mathbf{x}_{t+1}\in[0,1)^d} \|\mathcal{M}_{t+1,\widehat{\mathbb{Q}}_t^N}(\mathbf{x}_{t+1},\mathrm{d}\mathbf{x}_t) - \mathcal{M}_{t+1,\mathbb{Q}_t}(\mathbf{x}_{t+1},\mathrm{d}\mathbf{x}_t)\|_{\mathrm{E}} \\
&= o(1)
\end{aligned}$$

using (2.32). This complete the proof of (2.44).

We are now ready to prove the second statement of the theorem. Note that (2.33) is true for $t = 1$ by (2.44). Let $t > 1$ and $B_{0:t} \in \mathcal{B}_{[0,1)^d}^{t+1}$. Then,

$$\begin{aligned}
&\left|\int_{B_{0:t}} \left(\widetilde{\mathbb{Q}}_t^N - \widetilde{\mathbb{Q}}_t\right)(\mathrm{d}\mathbf{x}_{1:t})\right| = \left|\int_{B_{0:t}} \left(\widehat{\mathbb{Q}}_t^N \otimes \mathcal{M}_{t,\widehat{\mathbb{Q}}_{t-1}^N}(\mathrm{d}\mathbf{x}_{t-1:t}) \prod_{s=1}^{t-1} \mathcal{M}_{s,\widehat{\mathbb{Q}}_{s-1}^N}(\mathbf{x}_s,\mathrm{d}\mathbf{x}_{s-1})\right.\right. \\
&\left.\left. - \mathbb{Q}_t \otimes \mathcal{M}_{t,\mathbb{Q}_{t-1}}(\mathrm{d}\mathbf{x}_{t-1:t}) \prod_{s=1}^{t-1} \mathcal{M}_{s,\mathbb{Q}_{s-1}}(\mathbf{x}_s,\mathrm{d}\mathbf{x}_{s-1})\right)\right| \\
&\leq \left|\int_{B_{t-1:t}} \left[\int_{B_{0:t-2}} \prod_{s=1}^{t-1} \mathcal{M}_{s,\mathbb{Q}_{s-1}}(\mathbf{x}_s,\mathrm{d}\mathbf{x}_{s-1})\right] \left(\widehat{\mathbb{Q}}_t^N \otimes \mathcal{M}_{t,\widehat{\mathbb{Q}}_{t-1}^N} - \mathbb{Q}_t \otimes \mathcal{M}_{t,\mathbb{Q}_{t-1}}\right)(\mathrm{d}\mathbf{x}_{t-1:t})\right| \\
&+ \left|\int_{B_{t-1:t}} \widehat{\mathbb{Q}}_t^N \otimes \mathcal{M}_{t,\widehat{\mathbb{Q}}_{t-1}^N}(\mathrm{d}\mathbf{x}_{t-1:t}) \left(\int_{B_{0:t-2}} \prod_{s=1}^{t-1} \mathcal{M}_{s,\widehat{\mathbb{Q}}_{s-1}^N}(\mathbf{x}_s,\mathrm{d}\mathbf{x}_{s-1}) - \int_{B_{0:t-2}} \prod_{s=1}^{t-1} \mathcal{M}_{s,\mathbb{Q}_{s-1}}(\mathbf{x}_s,\mathrm{d}\mathbf{x}_{s-1})\right)\right|.
\end{aligned}$$

The first term after the inequality sign can be rewritten as

$$\left|\int_{B_{t-1:t}} \lambda_{(t-1)d}\left(F_{\otimes_{s=1}^{t-1}\mathcal{M}_{s,\mathbb{Q}_{s-1}}}(\mathbf{x}_{t-1},B_{0:t-2})\right)\left(\widehat{\mathbb{Q}}_t^N \otimes \mathcal{M}_{t,\widehat{\mathbb{Q}}_{t-1}^N} - \mathbb{Q}_t \otimes \mathcal{M}_{t,\mathbb{Q}_{t-1}}\right)(\mathrm{d}\mathbf{x}_{t-1:t})\right|.$$

The supremum of this quantity over $B_{0:t} \in \mathcal{B}_{[0,1)^d}^{t+1}$ is $o(1)$ using (2.44), the fact that $F_{\otimes_{s=1}^{t-1}\mathcal{M}_{s,\mathbb{Q}_{s-1}}}$ is Hölder continuous (because $F_{\mathcal{M}_{s,\mathbb{Q}_{s-1}}}$ is Hölder continuous for all s) and Lemma 2.1.

To control the second term we first prove by induction that, for any $t > 1$,

$$\sup_{B_{0:t-2}\in\mathcal{B}_{[0,1)^d}^{t-1}} \left|\int_{B_{0:t-2}} \prod_{s=1}^{t-1} \mathcal{M}_{s,\widehat{\mathbb{Q}}_{s-1}^N}(\mathbf{x}_s,\mathrm{d}\mathbf{x}_{s-1}) - \int_{B_{0:t-2}} \prod_{s=1}^{t-1} \mathcal{M}_{s,\mathbb{Q}_{s-1}}(\mathbf{x}_s,\mathrm{d}\mathbf{x}_{s-1})\right| = o(1) \tag{2.45}$$

uniformly on $\mathbf{x}_{t-1}$. By (2.32) this result is true for $t = 2$. Assume that (2.45) holds for $t > 2$. Then

$$\begin{aligned}
&\left| \int_{B_{0:t-1}} \prod_{s=1}^{t} \mathcal{M}_{s,\widehat{\mathbb{Q}}^N_{s-1}}(\mathbf{x}_s, \mathrm{d}\mathbf{x}_{s-1}) - \int_{B_{0:t-1}} \prod_{s=1}^{t} \mathcal{M}_{s,\mathbb{Q}_{s-1}}(\mathbf{x}_s, \mathrm{d}\mathbf{x}_{s-1}) \right| \\
&= \left| \int_{B_{0:t-1}} \left[\mathcal{M}_{t,\widehat{\mathbb{Q}}^N_{t-1}}(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t-1}) \prod_{s=1}^{t-1} \mathcal{M}_{s,\widehat{\mathbb{Q}}^N_{s-1}}(\mathbf{x}_s, \mathrm{d}\mathbf{x}_{s-1}) \right.\right. \\
&- \left.\left. \mathcal{M}_{t,\mathbb{Q}_{t-1}}(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t-1}) \prod_{s=1}^{t-1} \mathcal{M}_{s,\mathbb{Q}_{s-1}}(\mathbf{x}_s, \mathrm{d}\mathbf{x}_{s-1}) \right] \right| \\
&\leq \left| \int_{B_{t-1}} \mathcal{M}_{t,\widehat{\mathbb{Q}}^N_{t-1}}(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t-1}) \int_{B_{0:t-2}} \left(\prod_{s=1}^{t-1} \mathcal{M}_{s,\widehat{\mathbb{Q}}^N_{s-1}}(\mathbf{x}_s, \mathrm{d}\mathbf{x}_{s-1}) - \prod_{s=1}^{t-1} \mathcal{M}_{s,\mathbb{Q}_{s-1}}(\mathbf{x}_s, \mathrm{d}\mathbf{x}_{s-1}) \right) \right| \\
&+ \left| \int_{B_{t-1}} \lambda_{(t-1)d} \left(F_{\otimes_{s=1}^{t-1} \mathcal{M}_{s,\mathbb{Q}_{s-1}}}(\mathbf{x}_{t-1}, B_{0:t-2}) \right) \left(\mathcal{M}_{t,\widehat{\mathbb{Q}}^N_{t-1}}(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t-1}) - \mathcal{M}_{t,\mathbb{Q}_{t-1}}(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t-1}) \right) \right|
\end{aligned}$$

where we saw above that second term on the right side of the inequality sign is $o(1)$ uniformly on $\mathbf{x}_t$ while the first term is bounded by

$$\begin{aligned}
&\int_{[0,1)^d} \mathcal{M}_{t,\widehat{\mathbb{Q}}^N_{t-1}}(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t-1}) \\
&\times \sup_{B_{0:t-2} \in \mathcal{B}^{t-1}_{[0,1)^d}} \left| \int_{B_{0:t-2}} \left(\prod_{s=1}^{t-1} \mathcal{M}_{s,\widehat{\mathbb{Q}}^N_{s-1}}(\mathbf{x}_s, \mathrm{d}\mathbf{x}_{s-1}) - \prod_{s=1}^{t-1} \mathcal{M}_{s,\mathbb{Q}_{s-1}}(\mathbf{x}_s, \mathrm{d}\mathbf{x}_{s-1}) \right) \right|
\end{aligned}$$

where, by the inductive hypothesis, the second factor is $o(1)$ uniformly on $\mathbf{x}_{t-1} \in [0,1)^d$. This shows that (2.45) is true at time $t+1$ and therefore the proof of the theorem is complete.

D L_2-convergence: Theorem 2.2

To prove the result, let φ be as in the statement of the theorem and let us first prove the L_1-convergence.

We have

$$\mathbb{E}\left| \mathcal{S}(\tilde{\mathbf{x}}^{1:N}_{0:T})(\varphi) - \widetilde{\mathbb{Q}}_T(\varphi) \right| \leq \mathbb{E}\left| \mathcal{S}(\tilde{\mathbf{x}}^{1:N}_{0:T})(\varphi) - \widetilde{\mathbb{Q}}^N_T(\varphi) \right| + \mathbb{E}\left| \widetilde{\mathbb{Q}}^N_T(\varphi) - \widetilde{\mathbb{Q}}_T(\varphi) \right|.$$

By portmanteau lemma (Van der Vaart, 2007, Lemma 2.2, p.6), the convergence in the sense of the extreme metric is stronger than the weak convergence. Hence, the second term above goes to 0 as $N \to +\infty$ by Theorem 2.1 and by the dominated

convergence theorem. For the first term, as each $\tilde{\mathbf{u}}^n \sim \mathcal{U}([0,1)^{T+1})$, we have, by the inverse Rosenblatt interpretation of the backward pass of SQMC,

$$\mathbb{E}\Big[\mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N})(\varphi)\big|\mathcal{F}_T\Big] = \mathbb{E}\Big[\mathcal{S}(\tilde{h}_{0:T}^{1:N})(\varphi \circ H_T)\big|\mathcal{F}_T\Big] = \widetilde{\mathbb{Q}}_{T,h_T}^N(\varphi \circ H_T) = \widetilde{\mathbb{Q}}_T^N(\varphi)$$

with$\mathcal{F}_T^N$ the σ-algebra generated by the forward step (Algorithm 2.1). Therefore,

$$\mathbb{E}\left|\mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N})(\varphi) - \widetilde{\mathbb{Q}}_T^N(\varphi)\big|\mathcal{F}_T\right| \leq \mathrm{Var}\left(\mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N})(\varphi)\big|\mathcal{F}_T\right)^{1/2}$$

where, using Assumption 2 and the fact that $\tilde{\mathbf{x}}_{0:T}^n = H_T \circ F^{-1}_{\widetilde{\mathbb{Q}}^N_{T,h_T}}(\tilde{\mathbf{u}}^n)$,

$$\mathrm{Var}\left(\mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N})(\varphi)|\mathcal{F}_T^N\right) \leq \frac{c}{N}\sigma_{\varphi,N}^2$$

with $\sigma_{\varphi,N}^2 \leq \widetilde{\mathbb{Q}}_T^N(\varphi^2)$. Let $\epsilon > 0$. Then, by Assumption 1 and looking at the proof of Theorem 2.1, we have for N large enough and almost surely, $\widetilde{\mathbb{Q}}_T^N(\varphi^2) \leq \widetilde{\mathbb{Q}}_T(\varphi^2) + \epsilon$ so that, for N large enough,

$$\mathbb{E}\left|\mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N})(\varphi) - \widetilde{\mathbb{Q}}_T^N(\varphi)\right| \leq \sqrt{\frac{\widetilde{\mathbb{Q}}_T(\varphi^2) + \epsilon}{N}} \tag{2.46}$$

showing the L_1-convergence. To prove the L_2-convergence, remark that

$$\mathbb{E}\left[\mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N})(\varphi)|\mathcal{F}_T^N\right] = \widetilde{\mathbb{Q}}_T^N(\varphi) = (\widetilde{\mathbb{Q}}_T^N(\varphi) - \widetilde{\mathbb{Q}}_T(\varphi)) + \widetilde{\mathbb{Q}}_T(\varphi)$$

and therefore

$$\mathrm{Var}\Big(\mathbb{E}\Big[\mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N})(\varphi)|\mathcal{F}_T^N\Big]\Big) = \mathrm{Var}\Big(\widetilde{\mathbb{Q}}_T^N(\varphi) - \widetilde{\mathbb{Q}}_T(\varphi)\Big) \leq \mathbb{E}\Big[\big(\widetilde{\mathbb{Q}}_T^N(\varphi) - \widetilde{\mathbb{Q}}_T(\varphi)\big)^2\Big]$$

where the right-hand side converges to zero as $N \to +\infty$ by the dominated convergence theorem and by Theorem 2.1. On conclude the prove using (2.46) and the fact that

$$\mathrm{Var}\Big(\mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N})(\varphi)\Big) = \mathrm{Var}\Big(\mathbb{E}\Big[\mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N})(\varphi)|\mathcal{F}_T^N\Big]\Big) + \mathbb{E}\Big[\mathrm{Var}\Big(\mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N})(\varphi)|\mathcal{F}_T^N\Big)\Big].$$

E Consistency of the Backward step: Theorem 2.3 and Corollary 2.1

E.1 Preliminary computations

We first prove the following Lemma:

Lemma 2.1. *Let $m \in \mathbb{N}$, $I = [0, \frac{k+1}{2^{dm}}]$, $k \in \{0, 1, ..., 2^{dm} - 2\}$ and $B = H(I)$. Then, $B = \cup_{i=1}^{p} B_i$ for some closed hyperrectangles $B_i \subseteq [0,1]^d$ and where $p \leq 2^d(m+1)$.*

Proof. To prove the Lemma, let $0 \leq m_1 \leq m$ be the smallest integer $\tilde{m}$ such that $I^d_{\tilde{m}}(0) \subseteq I$ and $i^*_{m_1}$ be the number of intervals in $\mathcal{I}^d_{m_1}$ included in I. Note that $i^*_{m_1} < 2^d$. Indeed, if $i^*_{m_1} \geq 2^d$ then, by the nesting property of the Hilbert curve,

$$I^d_{m_1-1}(0) \subseteq \bigcup_{k=0}^{d-1} I^d_{m_1}(k) \subseteq \bigcup_{k=0}^{i^*_{m_1}-1} I^d_{m_1}(k) \subseteq I$$

which is in contradiction with the definition of $i^*_{m_1}$. Define $I_2 = I \setminus \cup \mathcal{I}^I_{m_1}$ and $i^*_{m_2}$ the number of intervals in $\mathcal{I}^d_{m_2}$ included in I_2. For the same reason as above $i^*_{n_2} < 2^d$. More generally, for any $m_1 \leq m_k \leq m$, $i^*_{m_k} \leq 2^d$ meaning that the set B is made of at most $\sum_{k=m_1}^{m} i^*_{m_k} \leq 2^d(m+1)$ hypercubes (of side varying between 2^{-m} and 2^{-m_1}). □

The second result we need to prove Theorem 2.3 is an extension of Gerber and Chopin (2014, Theorem 3) and of Theorem 2.3 above for the mapping h_T for the case $T > 1$.

Lemma 2.2.

1. *Let $(\pi^N)_{N\geq 1}$ be a sequence of probability measure on $[0,1)^{(T+1)d}$ such that $\|\pi^N - \pi\|_{\mathrm{E}} \to 0$ where $\pi(\mathrm{d}\mathbf{x}) = \pi(\mathbf{x})\lambda_{(T+1)d}(\mathrm{d}\mathbf{x})$ is a probability measure on $\pi^{(T+1)d}$ that admits a bounded density $\pi(\mathbf{x})$. Let π_{h_T} be the image by h_T of π. Then,*

$$\|\pi^N_{h_T} - \pi_{h_T}\|_{\mathrm{E}} \to 0, \quad \text{as } N \to +\infty.$$

2. *Let $\pi(\mathrm{d}\mathbf{x})$ and π_{h_T} be as in 2. and $(\pi^N_{h_T})_{N\geq 1}$ a sequence of probability measures on $[0,1)^{(T+1)}$ such that $\|\pi^N_{h_T} - \pi_{h_T}\|_{\mathrm{E}} \to 0$ as $N \to +\infty$. Let π^N be the image by H_T of $\pi^N_{h_T}$. Then,*

$$\|\pi^N - \pi\|_{\mathrm{E}} \to 0, \quad \text{as } N \to +\infty.$$

The proof of this lemma is omitted since it follows from the properties of Cartesian products and from straightforward modifications of the proof of Gerber and Chopin (2014, Theorem 3) and of Theorem 2.3 above.

E.2 Proof of the Theorem

To prove the theorem first note that

$$\|\widetilde{\mathbb{Q}}^N_{T,h_T} - \widetilde{\mathbb{Q}}_{T,h_T}\|_{\mathrm{E}} = o(1).$$

Indeed, by assumption, $\|\widehat{\mathsf{Q}}^N_{T,h} - \widehat{\mathbb{Q}}^N_{T,h}\|_{\mathrm{E}} = o(1)$ and, by Theorem 2.1 and Lemma 2.2 (part 1 with $T = 1$), $\|\widehat{\mathbb{Q}}^N_{T,h} - \mathbb{Q}_{T,h}\|_{\mathrm{E}} = o(1)$ since $\mathbb{Q}_T$ admits a bounded density (Assumption 4 of Theorem 2.1). Hence, $\|\widehat{\mathsf{Q}}^N_{T,h} - \mathbb{Q}_{T,h}\|_{\mathrm{E}} = o(1)$. Let $\widehat{\mathsf{Q}}^N_T$ be the image by H of $\widehat{\mathsf{Q}}^N_{T,h}$. Then, $\|\widehat{\mathsf{Q}}^N_T - \mathbb{Q}_T\|_{\mathrm{E}} = o(1)$ by Theorem 2.3. Using the same argument, and using the fact that, for all $t \in 1 : T$, $\tilde{G}_t$ is bounded (Assumption H2 of Theorem 2.1), it is easy to show that, for any $t \in 0 : T$,

$$\sup_{\mathbf{x}_t \in \mathcal{X}} \|K^N_t(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t-1}) - \mathcal{M}_{t,\mathbb{Q}_{t-1}}(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t-1})\|_{\mathrm{E}} = o(1)$$

where we write $K^N_t(\mathbf{x}_t, \mathrm{d}\mathbf{x}_{t-1})$ the image by H of the probability measure $K_{t,h}(H(\mathbf{x}_t), \mathrm{d}h_{t-1})$. Hence, by the second part of Theorem 2.1, $\|\widetilde{\mathsf{Q}}^N_T - \widetilde{\mathbb{Q}}_T\|_{\mathrm{E}} = o(1)$ where $\widetilde{\mathsf{Q}}^N_T$ denotes the image by H_T of $\widetilde{\mathsf{Q}}^N_{T,h_T}$. Finally, under the assumptions of the theorem, $\widetilde{\mathbb{Q}}_T$ admits a bounded density (because for all t, $\tilde{G}_t$ is bounded and $\mathbb{Q}_t$ admits a bounded density) and thus, by Lemma 2.2 (part 1), $\|\widetilde{\mathsf{Q}}^N_{T,h_T} - \widetilde{\mathbb{Q}}_{T,h_T}\|_{\mathrm{E}} = o(1)$.

Consequently, to prove the theorem it remains to show that

$$\|\mathcal{S}(\check{h}^{1:N}_{0:T}) - \widetilde{\mathsf{Q}}^N_{T,h_T}\|_{\mathrm{E}} = o(1). \tag{2.47}$$

Indeed, this would yield $\|\mathcal{S}(\check{h}^{1:N}_{0:T}) - \widetilde{\mathbb{Q}}_{T,h_T}\|_{\mathrm{E}} = o(1)$ and therefore, by Lemma 2.2 (part 2), $\|\mathcal{S}(\check{\mathbf{x}}^{1:N}_{0:T}) - \widetilde{\mathbb{Q}}_T\|_{\mathrm{E}} = o(1)$.

To prove (2.47), we assume to simplify the notations that $F_{\mathcal{M}_{t,\mathbb{Q}_{t-1}}}(\mathbf{x}_t, \mathbf{x}_{t-1})$ is Lipschitz. Generalization for any Hölder exponent can be done using similar arguments as in the proof of Theorem 2.2.

Let $h^n_t = h(\mathbf{x}^N_t)$ where $\mathbf{x}^{1:N}_t$ are the particles obtained at the end of iteration t of Algorithm 2.1. We assume that for all $t \in 0 : T$ the particles are sorted according to their Hilbert index, i.e. $n < m \implies h^n_t < h^m_t$ (note that the inequality is strict by Assumption 1 of Theorem 2.1). Then, one has

$$\|\mathcal{S}(\check{h}^{1:N}_{0:T}) - \widetilde{\mathsf{Q}}^N_{T,h_T}\|_{\mathrm{E}} = \sup_{B \in \mathcal{B}^N_{[0,1)^{T+1}}} \left|\alpha_N\left(F_{\widetilde{\mathsf{Q}}^N_{T,h_T}}(B)\right) - \lambda_{T+1}\left(F_{\widetilde{\mathsf{Q}}^N_{T,h_T}}(B)\right)\right|$$

where $\mathcal{B}^N_{[0,1)^{T+1}} = \left\{[\boldsymbol{a}, \boldsymbol{b}] \subset \mathcal{B}_{[0,1)^{T+1}},\, b^N_i \le h^N_i,\, i \in 0 : T\right\}$.

The beginning of the proof follows the lines of Theorem 2.2, with $\beta = d$ and d replaced by $T + 1$. Let $\tilde{d} = \sum_{t=0}^T d^t$ so that, for a set $B \in \mathcal{B}^N_{[0,1)^{T+1}}$,

$$\left|\alpha_N\left(F_{\widetilde{\mathsf{Q}}^N_{T,h_T}}(B)\right) - \lambda_{T+1}\left(F_{\widetilde{\mathsf{Q}}^N_{T,h_T}}(B)\right)\right| \le L^{\tilde{d}} D(\mathbf{u}^{1:N}) + \#\mathcal{U}_2\left\{D(\mathbf{u}^{1:N}) + L^{-\tilde{d}}\right\}$$

where L and $\mathcal{U}_2$ are as in the proof of Theorem 2.2.

Following this latter, let $\mathcal{P}'$ be the partition of the set $[0,1)^{T+1}$ into hyperrectangles W' of size $L'^{-d^T} \times L'^{-d^{T-1}} \times ... \times L'^{-1}$ such that, for all $\boldsymbol{h}$ and $\boldsymbol{h}'$ in W', we have

$$|F_{\widehat{\mathsf{Q}}^N_{T,h}}(h_1) - F_{\widehat{\mathsf{Q}}^N_{T,h}}(h'_1)| \le L^{-d^T}. \tag{2.48}$$

and

$$\left|\tilde{F}^N_{i-1}(h_{i-1},h_i)-\tilde{F}^N_{i-1}(h'_{i-1},h'_i)\right|\leq L^{-d^{T+1-i}},\quad i\in 2:(T+1) \tag{2.49}$$

where, to simplify the notations, we write $\tilde{F}^N_{i-1}(h_1,\cdot)$ the CDF of $K^N_{T-i+2,h}(h_1,\mathrm{d}h_{T-i+1})$.

Let us first look at condition (2.48). We have

$$\begin{aligned}|F_{\widehat{\mathbb{Q}}^N_{T,h}}(h_1)-F_{\widehat{\mathbb{Q}}^N_{T,h}}(h'_1)|&\leq 2\|F_{\widehat{\mathbb{Q}}^N_{T,h}}-F_{\widehat{\mathbb{Q}}^N_{T,h}}\|_\infty+2\|F_{\widehat{\mathbb{Q}}^N_{T,h}}-F_{\mathbb{Q}_{T,h}}\|_\infty+|F_{\mathbb{Q}_{T,h}}(h_1)-F_{\mathbb{Q}_{T,h}}(h'_1)|\\&\leq 2r_1(N)+2r_2(N)+\left|F_{\mathbb{Q}_{T,h}}(h_1)-F_{\mathbb{Q}_{T,h}}(h'_1)\right|\end{aligned}$$

with $r_1(N)=\|F_{\widehat{\mathbb{Q}}^N_{T,h}}-F_{\widehat{\mathbb{Q}}^N_{T,h}}\|_\infty$, $r_2(N)=\|\widehat{\mathbb{Q}}^N_{T,h}-\mathbb{Q}_{T,h}\|_{\mathrm{E}}$; note $r_1(N)\to 0$ by construction and under the assumptions of the theorem while $r_2(N)\to 0$ by Theorem 2.1 and by Lemma 2.2.

Let $L'=2^m$ for an integer $m\geq 0$, so that h_i and h'_i are in the same interval $I^d_{d^{T-i}m}(k)\in\mathcal{I}^d_{d^{T-i}m}$, $i\in 1:(T+1)$. Then, since h_1 and h'_1 are in the same interval $I^d_{d^{T-1}m}(k)\in\mathcal{I}^d_{d^{T-1}m}$,

$$\left|F_{\mathbb{Q}_{T,h}}(h_1)-F_{\mathbb{Q}_{T,h}}(h'_1)\right|\leq\mathbb{Q}_{T,h}\left(I^d_{d^{T-1}m}(k)\right)=\mathbb{Q}_T\left(S^d_{d^{T-1}m}(k)\right)\leq\frac{\|p_T\|_\infty}{(L')^{d^T}}$$

as $\mathbb{Q}_T$ admits a bounded density p_T. Hence (2.48) is verified if

$$L'\geq L\tilde{k}_N,\quad \tilde{k}_N=\left(\frac{\|p_T\|_\infty}{(1-L^{d^T}r^*_1(N))}\right)^{1/d^T},\quad r^*_1(N)=2r_1(N)+2r_2(N),$$

which implies that we assume from now on that $L^{-d^T}\geq 2r^*_1(N)$ for N large enough.

Let us now look at (2.49) for a $i>1$. To simplify the notations in what follows, let $F^N_{i-1}(h_1,\cdot)$ be the CDF of $\mathcal{M}^h_{T-i+2,\widehat{\mathbb{Q}}^N_{T-i+1,h}}(h_1,\mathrm{d}h_{T-i+1})$ and $F_{i-1}(h_1,\cdot)$ be the CDF of $\mathcal{M}^h_{T-i+2,\mathbb{Q}_{T-i+1}}(h_1,\mathrm{d}h_{T-i+1})$. Then,

$$\begin{aligned}&\left|\tilde{F}^N_{i-1}(h_{i-1},h_i)-\tilde{F}^N_{i-1}(h'_{i-1},h'_i)\right|\\&\leq 2\|\tilde{F}^N_{i-1}-F^N_{i-1}\|_\infty+2\|F^N_{i-1}-F_{i-1}\|_\infty+|F_{i-1}(h_{i-1},h_i)-F_{i-1}(h'_{i-1},h'_i)|\\&=2r_3(N)+2r_4(N)+\left|F_{i-1}(h_{i-1},h_i)-F_{i-1}(h'_{i-1},h'_i)\right|\end{aligned}$$

with $r_3(N)=\|\tilde{F}^N_{i-1}-F^N_{i-1}\|_\infty$, $r_4(N)=\|F^N_{i-1}-F_{i-1}\|_\infty$; note $r_3(N)\to 0$ by construction and under the assumptions of the theorem while $r_4(N)\to 0$ by Theorem 2.1 and Lemma 2.2.

To control $\left|F_{i-1}(h_{i-1},h_i)-F_{i-1}(h'_{i-1},h'_i)\right|$, assume without loss of generality that $h_i>h'_i$ and write $\tilde{G}^h_i(h_{i-1},h'_i)=\tilde{G}_{T-i+2}(H(h_{i-1}),H(h'_i))$ to simplify he notations. Then

$$\begin{aligned}|F_{i-1}(h_{i-1},h_i)-F_{i-1}(h'_{i-1},h'_i)|&\leq|F_{i-1}(h_{i-1},h'_i)-F_{i-1}(h'_{i-1},h'_i)|\\&\quad+\left|\int_{h'_i}^{h_i}\tilde{G}^h(h_{i-1},v)\mathbb{Q}_{T-i+1,h}(\mathrm{d}v)\right|.\end{aligned}$$

The second term is bounded by $\|\tilde{G}_{T-i+2}\|_\infty \mathbb{Q}_{T-i+1,h}([h'_i, h_i]) \leq \|\tilde{G}_{T-i+2}\|_\infty \mathbb{Q}_{T-i+1}(W)$ where $W \in \mathcal{S}^d_{d^{T-i}m}$. Since $\mathbb{Q}_{T-i+1}$ admits a bounded density, we have, for a constant $c > 0$,

$$\|\tilde{G}_{T-i+2}\|_\infty \mathbb{Q}_{T-i+1,h}([h'_i, h_i]) \leq cL^{-d^{T+1-i}}.$$

To control the other term suppose first that $h'_i > L'^{-d^{T-i+1}}$ and let k be the largest integer such that $h'_i \geq kL'^{-d^{T-i+1}}$. Then,

$$\begin{aligned}
&\left| \int_0^{h'_i} \left[\tilde{G}^h_i(h_{i-1}, v) - \tilde{G}^h_i(h'_{i-1}, v) \right] \mathbb{Q}_{T-i+1,h}(\mathrm{d}v) \right| \leq \\
&\left| \int_0^{kL'^{-d^{T-i+1}}} \left[\tilde{G}^h_i(h_{i-1}, v) - \tilde{G}^h_i(h'_{i-1}, v) \right] \mathbb{Q}_{T-i+1,h}(\mathrm{d}v) \right| + \\
&\left| \int_{kL'^{-d^{T-i+1}}}^{h'_i} \left[\tilde{G}^h_i(h_{i-1}, v) - \tilde{G}^h_i(t'_{i-1}, v) \right] \mathbb{Q}_{T-i+1,h}(\mathrm{d}v) \right|.
\end{aligned} \tag{2.50}$$

Then, using by Lemma 2.1, the first term after the inequality sign term of (2.50) can be bounded as follows:

$$\begin{aligned}
&\left| \sum_{j=1}^{k_i} \int_{W_j} \left[\tilde{G}_{T-i+2}(H(h_{i-1}), \mathbf{x}) - \tilde{G}_{T-i+2}(H(h'_{i-1}), \mathbf{x}) \right] \mathbb{Q}_{T-i+1}(\mathrm{d}\mathbf{x}) \right| \\
&\leq \sum_{j=1}^{k_i} \left\{ \left| F^{cdf}_{\mathcal{M}_{T-i+2,\mathbb{Q}_{T-i+1}}}(H(h_{i-1}), \mathbf{a_j}) - F^{cdf}_{\mathcal{M}_{T-i+2,\mathbb{Q}_{T-i+1}}}(H(h'_{i-1}), \mathbf{a_j}) \right| \right. \\
&\left. + \left| F^{cdf}_{\mathcal{M}_{T-i+2,\mathbb{Q}_{T-i+1}}}(H(h_{i-1}), \mathbf{b_j}) - F^{cdf}_{\mathcal{M}_{T-i+2,\mathbb{Q}_{T-i+1}}}(H(h'_{i-1}), \mathbf{b_j}) \right| \right\}
\end{aligned}$$

where $W_j = [\mathbf{a}_j, \mathbf{b_j}] \subset [0,1)^d$ and where $k_i \leq 2^d(d^{T-i}m + 1)$. Let C_i be the Lipschitz constant of $F^{cdf}_{\mathcal{M}_{T-i+2,\mathbb{Q}_{T-i+1}}}$. Then, for any $\mathbf{c} \in [0,1)^d$,

$$\begin{aligned}
\left| F^{cdf}_{\mathcal{M}_{T-i+2,\mathbb{Q}_{T-i+1}}}(H(h_{i-1}), \mathbf{c}) - F^{cdf}_{\mathcal{M}_{T-i+2,\mathbb{Q}_{T-i+1}}}(H(h'_{i-1}), \mathbf{c}) \right| &\leq C_i \|H(h_{i-1}) - H(h'_{i-1})\|_\infty \\
&\leq C_i L'^{-d^{T-i+1}}
\end{aligned}$$

because $H(h_{i-1})$ and $H(h'_{i-1})$ belong to the same hypercube $W \in \mathcal{S}^d_{d^{T-i+1}m}$ of side $2^{-md^{T-i+1}} = L'^{-d^{T-i+1}}$.

For the second term after the inequality sign in (2.50), we have

$$\begin{aligned}
&\left| \int_{kL'^{-d^{T-i+1}}}^{h'_i} \left[\tilde{G}^h_i(h_{i-1}, v) - \tilde{G}^h_i(h'_{i-1}, v) \right] \mathbb{Q}_{T-i+1,h}(\mathrm{d}v) \right| \\
&\leq \mathcal{M}^h_{T-i+2,\mathbb{Q}_{T-i+1},h}(h_{i-1}, [kL'^{-d^{T-i+1}}, h'_i]) + \mathcal{M}^h_{T-i+2,\mathbb{Q}_{T-i+1},h}(h'_{i-1}, [kL'^{-d^{T-i+1}}, h'_i]) \\
&\leq \mathcal{M}_{T-i+2,\mathbb{Q}_{T-i+1}}(H(h_{i-1}), W) + \mathcal{M}_{T-i+2,\mathbb{Q}_{T-i+1}}(H(h'_{i-1}), W) \\
&\leq 2\|\tilde{G}_{T-i+2}\|_\infty \|p_{T-i+1}\|_\infty 2^{-md^{T-i+1}}
\end{aligned}$$

for a $W \in \mathcal{S}^d_{d^{T-i}m}$ and where p_{T-i+1} is the (bounded) density of $\mathbb{Q}_{T-i+1}$. This last quantity is also the bound we obtain for $h'_i < L'^{-d^{T-i+1}}$. Hence, these computations shows that

$$|\tilde{F}_{i-1}(h_{i-1}, h_i) - \tilde{F}_{i-1}(h'_{i-1}, h'_i)| \leq c_i L'^{-d^{T-i+1}} \log(L')$$

for a constants c_i, $i \in 2 : (T+1)$.

Condition (2.49) is therefore verified when

$$\frac{L'}{\log(L')} \geq L \max_{i \in \{2,\dots,T+1\}} \left(\frac{c_i}{1 - L^{d^{T-i+1}} r_2^*(N))} \right)^{\frac{1}{d^{T-i+1}}}$$

where $r_2^*(N) = 2r_3(N) + 2r_4(N)$. Let $\gamma \in (0,1)$ and note that for N large enough $\log L' < L'^{\gamma}$. Hence, for N large enough (2.48) and (2.49) are verified for L' the smallest power of 2 such that

$$L' \geq (k_N L)^{(1-\gamma)^{-1}}, \quad k_N = \max_{i \in \{1,\dots,T+1\}} \left(\frac{c_i}{1 - L^{d^{T-i+1}} r^*(N))} \right)^{\frac{1}{d^{T-i+1}}}, \quad c_1 = \|p_T\|$$

where $r^*(N) = r_1^*(N) + r_2^*(N)$. Note that we assume from now on that $L^{-d^T} \geq 2r^*(N)$.

Because the function $F_{\widetilde{\mathbb{Q}}^N_{T,h_T}}$ is continuous on $[0, h_0^N] \times \cdots \times [0, h_T^N]$, $\partial(F_{\widetilde{\mathbb{Q}}^N_{T,h_T}}(B)) = F_{\widetilde{\mathbb{Q}}^N_{T,h_T}}(\partial(B))$ and therefore we can bound $\#\mathcal{U}_2$ following the proof of Theorem 2.2. Using the same notations as in the proof of Theorem 2.2, we obtain that $\widetilde{\mathbb{Q}}^N_{T,h_T}(\partial(B))$ is covered by at most

$$(T+1)2^{\tilde{d}} k_N^{\frac{\tilde{d}-1}{1-\gamma}} L^{\frac{\tilde{d}-1}{1-\gamma}}$$

hyperrectangles in $\tilde{\mathcal{R}}$. To go back to the initial partition of $[0,1)^{T+1}$ with hyperrectangles $W \in \mathcal{P}$, remark that $L' > L$ so that every hyperrectangles in $\tilde{\mathcal{R}}$ is covered by at most c^* hyperrectangles of $\mathcal{P}$ for a constant c^*. Hence,

$$\#\mathcal{U}_2^{(1)} \leq c_N L^{\frac{\tilde{d}-1}{1-\gamma}}, \quad c_N = c^*(T+1)2^{\tilde{d}} k_N^{\frac{\tilde{d}-1}{1-\gamma}}. \tag{2.51}$$

We therefore have

$$\|\mathcal{S}(\check{h}^{1:N}_{0:T}) - \widetilde{\mathbb{Q}}^N_{T,h_T}\|_{\mathrm{E}} \leq L^{\tilde{d}} D(\mathbf{u}^{1:N}) + c_N L^{\frac{\tilde{d}-1}{1-\gamma}} \left(D(\mathbf{u}^{1:N}) + L^{-\tilde{d}} \right).$$

Let $\gamma \in (0, \tilde{d}^{-1})$ so that $c_d := \tilde{d} - \frac{\tilde{d}-1}{1-\gamma} > 0$. To conclude the proof as in Gerber and Chopin (2014, Theorem 4), let $\tilde{d}_1 = d^T$ and $\tilde{d}_2 = \sum_{t=0}^{T-1} d^t$. Thus,

$$\|\mathcal{S}(\check{h}^{1:N}_{0:T}) - \widetilde{\mathbb{Q}}^N_{T,h_T}\|_{\mathrm{E}} \leq 2L^{\tilde{d}_1 + \tilde{d}_2} D(\mathbf{u}^{1:N}) + L^{-c_d}$$

where the optimal value of L is such that $L = \mathcal{O}(D(\mathbf{u}^{1:N})^{-\frac{1}{c_d+\tilde{d}_1+\tilde{d}_2}})$. Then, provided that $r^*(N)D(\mathbf{u}^{1:N})^{-\frac{\tilde{d}_1}{c_d+\tilde{d}_1+\tilde{d}_2}} = \mathcal{O}(1)$, L verifies all the conditions above and, since $c_N = \mathcal{O}(1)$, we have

$$\|\mathcal{S}(\check{h}_{0:T}^{1:N}) - \widetilde{\mathsf{Q}}_{T,h_T}^N\|_{\mathrm{E}} = \mathcal{O}\left(D(\mathbf{u}^{1:N})^{\frac{1}{c_d+\tilde{d}_1+\tilde{d}_2}}\right).$$

Otherwise, if $r^*(N)D(\mathbf{u}^{1:N})^{-\frac{\tilde{d}_1}{c_d+\tilde{d}_1+\tilde{d}_2}} \to +\infty$, let $L = \mathcal{O}(r^*(N)^{-\frac{1}{\tilde{d}_1}})$. Then $c_N = \mathcal{O}(1)$ and

$$\begin{aligned} L^{\tilde{d}_1+\tilde{d}_2}D(\mathbf{u}^{1:N}) &= \mathcal{O}(r(N))^{\frac{c_d}{\tilde{d}_1}-\frac{c_d+\tilde{d}_1+\tilde{d}_2}{\tilde{d}1}}D(\mathbf{u}^{1:N}) \\ &= \mathcal{O}(r(N)^{c_d/\tilde{d}_1})\left(\mathcal{O}(r(N))^{-1}D(\mathbf{u}^{1:N})^{\frac{\tilde{d}_1}{c_d+\tilde{d}_1+\tilde{d}_2}}\right)^{\frac{c_d+\tilde{d}_1+\tilde{d}_2}{\tilde{d}_1}} \\ &= \mathcal{o}\left(r(N)^{c_d/\tilde{d}_1}\right). \end{aligned}$$

Therefore $\|\mathcal{S}(\check{h}_{0:T}^{1:N}) - \widetilde{\mathsf{Q}}_{T,h_T}^N\|_{\mathrm{E}} = \mathcal{o}(1)$, which concludes the proof.

E.3 Proof of the Corollary 2.1

To prove the result we first construct a probability measure $\widetilde{\mathsf{Q}}_{T,h_T}^N$ such that the point set $\tilde{\mathbf{x}}_{0:T}^{1:N}$ generated by Algorithm 2.2 becomes, as N increases, arbitrary close to the point set $\check{\mathbf{x}}_{0:T}^{1:N}$ obtained using a smooth backward step which is as in Theorem 2.3. Then, we show that this implies that, if $\|\mathcal{S}(\check{\mathbf{x}}_{0:T}^{1:N}) - \widetilde{\mathbb{Q}}_T\|_{\mathrm{E}} \to 0$, then$\|\mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N}) - \widetilde{\mathbb{Q}}_T\|_{\mathrm{E}} \to 0$.

Assume that for all $t \in 0:T$ the points $h_t^{1:N}$ are labelled so that $n < m \implies h_t^n < h_t^m$. (Note that the inequality is strict because, by Assumption 1 of Theorem 2.1, the points $\mathbf{x}_t^{1:N}$ are distinct.) Without loss of generality, assume that $h_t^1 > 0$ and let $h_t^0 = 0$ for all t.

To construct $\widetilde{\mathsf{Q}}_{T,h_T}^N$, let $\widehat{\mathsf{Q}}_{T,h}^N$ be such that $F_{\widehat{\mathsf{Q}}_{T,h}^N}$ is strictly increasing on $[0, h_T^N]$ with $F_{\widehat{\mathsf{Q}}_{T,h}^N}(h_T^n) = F_{\widehat{\mathbb{Q}}_{T,h}^N}(h_T^n)$ for all $n \in 1:N$ and, for $t \in 1:T$, let $K_{t,h}^N(h_1, \mathrm{d}h_{t-1})$ be such, for all $n \in 1:N$ and for all $h_1 \in [0,1)$, $F_{K_{t,h}^N}(h_1, \cdot)$ is strictly increasing on $[0, h_{t-1}^N]$ and

$$F_{K_{t,h}^N}(h_1, h_{t-1}^n) = F_{\mathcal{M}_{t,\widehat{\mathbb{Q}}_{t-1,h}^N}^h}(h_1, h_{t-1}^n).$$

Let $\check{h}_{0:T}^{1:N}$ be as in Theorem 2.3 (with $\widetilde{\mathsf{Q}}_{T,h_T}^N$ constructed using the the above choice of $\widehat{\mathsf{Q}}_{T,h}^N$ and $K_{t,h}^N(h_1, \mathrm{d}h_{t-1})$). We now show by a backward induction that for any $t \in 0:T$, $\max_{n\in 1:N} \|\check{\mathbf{x}}_t^n - \tilde{\mathbf{x}}_t^n\|_\infty = \mathcal{o}(1)$.

To see this, note that, by the construction of $\widehat{\mathsf{Q}}_{T,h}^N$,

$$|\check{h}_T^n - \tilde{h}_T^n| \leq \Delta_T^N, \quad \Delta_T^N = \max_{n\in 1:N} |h_T^{n-1} - h_T^n|$$

where, by Gerber and Chopin (2014, Lemma 9), $\Delta_T^N \to 0$ as $N \to +\infty$. Hence, using the Hölder property of the Hilbert curve, this shows that $\max_{n\in 1:N} \|\check{\mathbf{x}}_T^n - \tilde{\mathbf{x}}_T^n\|_\infty = o(1)$.

Let $t \in 0:T-1$ and assume that $\max_{n\in 1:N} \|\check{\mathbf{x}}_{t+1}^n - \tilde{\mathbf{x}}_{t+1}^n\|_\infty = o(1)$. Let $w_t^n = h(\mathbf{x}_t^{\check{a}_t^n})$ where $\check{a}_t^n$ is the indices selected at iteration t of Algorithm 2.2 obtained by replacing $\tilde{\mathbf{x}}_{t+1}^n$ by $\check{\mathbf{x}}_{t+1}^n$. Then, by the construction of $K_{t,h}^N$, $\max_{n\in 1:N} |w_t^n - \check{h}_T^n| = o(1)$.

We now want to show that $\max_{n\in 1:N} |w_t^n - \tilde{h}_T^n| = o(1)$. To this purpose, let C_{t+1} and κ_{t+1} be respectively the Hölder constant and the Hölder exponent of m_{t+1}. Then,

$$\begin{aligned}|\widetilde{W}_t^i(\tilde{\mathbf{x}}_{t+1}^n) - \widetilde{W}_t^i(\check{\mathbf{x}}_{t+1}^n)| &\leq \|G_t\|_\infty \frac{|m_{t+1}(\mathbf{x}_t^i, \tilde{\mathbf{x}}_{t+1}^n) - m_{t+1}(\mathbf{x}_t^i, \check{\mathbf{x}}_{t+1}^n)|}{Nc_t} \\ &\leq \tilde{\xi}_t^N := \frac{\|G_t\|_\infty C_{t+1} \|\tilde{\mathbf{x}}_{t+1}^n - \check{\mathbf{x}}_{t+1}^n\|_\infty^{\kappa_{t+1}}}{Nc_t}\end{aligned}$$

where, by the inductive hypothesis, $\tilde{\xi}_t^N = o(N^{-1})$. Also, we know that

$$\min_{i\in 1:N} \inf_{\mathbf{x}_{t+1}\in\mathcal{X}} \widetilde{W}_t^i(\mathbf{x}_{t+1}) \geq \xi_t^N := \frac{\underline{G}_t \underline{m}_{t+1}}{N\|G_t\|_\infty \|m_{t+1}\|_\infty}.$$

Then, let N_t be such that $\tilde{\xi}_t^N < \xi_t^N$ so that, for $N \geq N_t$, we either have $\tilde{h}_t^n = w_t^n$, or $\tilde{h}_t^n = w_t^{n+1}$ or $\tilde{h}_t^n = w_t^{n-1}$. Hence, $\max_{n\in 1:N} |w_t^n - \tilde{h}_t^n| = o(1)$ and therefore $\max_{n\in 1:N} |\tilde{h}_t^n - \check{h}_t^n| = o(1)$. Finally, by, the Hölder property of the Hilbert curve, this shows that $\max_{n\in 1:N} \|\check{\mathbf{x}}_t^n - \tilde{\mathbf{x}}_t^n\|_\infty = o(1)$.

The rest of the proof follows the lines of Niederreiter (1992, Lemma 2.5, p.15). First, note that the above computations shows that for any $\epsilon > 0$ there exists a N_ϵ such that $\|\tilde{\mathbf{x}}_{0:T}^{1:N} - \check{\mathbf{x}}_{0:T}^{1:N}\|_\infty \leq \epsilon$. Let $B = [\boldsymbol{a}, \boldsymbol{b}]$, $B^+ = [\boldsymbol{a}, \boldsymbol{b} + \epsilon] \cap [0,1)^{T+1}$ and $B^- = [\boldsymbol{a}, \boldsymbol{b} - \epsilon]$. If $\epsilon > b_i$ for at least one $i \in 1:(T+1)$, $B^- = \varnothing$. Then for $N \geq N_\epsilon$, we have

$$\mathcal{S}(\check{\mathbf{x}}_{0:T}^{1:N})(B^-) \leq \mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N})(B) \leq \mathcal{S}(\check{\mathbf{x}}_{0:T}^{1:N})(B^+). \tag{2.52}$$

By the definition of the discrepancy, we have

$$\begin{aligned}\left|\mathcal{S}(\check{\mathbf{x}}_{0:T}^{1:N})(B^+) - \widetilde{\mathbb{Q}}_T(Q^+)\right| &\leq \|\mathcal{S}(\check{\mathbf{x}}_{0:T}^{1:N}) - \widetilde{\mathbb{Q}}_T\|_{\mathrm{E}}, \\ \left|\mathcal{S}(\check{\mathbf{x}}_{0:T}^{1:N})(B^-) - \widetilde{\mathbb{Q}}_T(B^-)\right| &\leq \|\mathcal{S}(\check{\mathbf{x}}_{0:T}^{1:N}) - \widetilde{\mathbb{Q}}_T\|_{\mathrm{E}}.\end{aligned} \tag{2.53}$$

Combining (2.52) and (2.53) yields:

$$\begin{cases} -\left(\widetilde{\mathbb{Q}}_T(B) - \widetilde{\mathbb{Q}}_T(B^-)\right) - \|\mathcal{S}(\check{\mathbf{x}}_{0:T}^{1:N}) - \widetilde{\mathbb{Q}}_T\|_{\mathrm{E}} \leq \mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N})(B) - \widetilde{\mathbb{Q}}_T(B) \\ \mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N})(B) - \widetilde{\mathbb{Q}}_T(B) \leq \left(\widetilde{\mathbb{Q}}_T(B^+) - \widetilde{\mathbb{Q}}_T(B)\right) + \|\mathcal{S}(\check{\mathbf{x}}_{0:T}^{1:N}) - \widetilde{\mathbb{Q}}_T\|_{\mathrm{E}}. \end{cases} \tag{2.54}$$

Using the fact that $\widetilde{\mathbb{Q}}_T$ admits a bounded density, we have for a constant $c > 0$

$$\begin{aligned} \widetilde{\mathbb{Q}}_T(B) - \widetilde{\mathbb{Q}}_T(B^-) &\leq c\lambda_{T+1}(B \setminus B^-) \leq c\,\epsilon^{T+1} \\ \widetilde{\mathbb{Q}}_T(B^+) - \widetilde{\mathbb{Q}}_T(B) &\leq c\lambda_{T+1}(B^+ \setminus B) \leq c\,\epsilon^{T+1} \end{aligned} \tag{2.55}$$

Therefore, combining (2.54) and (2.55), we obtain, for $N \geq N_\epsilon$ and for all $B \in \mathcal{B}_{[0,1)^{T+1}}$,

$$c\,\epsilon^{T+1} - \|\mathcal{S}(\check{\mathbf{x}}_{0:T}^{1:N}) - \widetilde{\mathbb{Q}}_T\|_{\mathrm{E}} \leq \mathcal{S}(\tilde{\mathbf{x}}_{0:T}^{1:N})(B) - \widetilde{\mathbb{Q}}_T(B) \leq \|\mathcal{S}(\check{\mathbf{x}}_{0:T}^{1:N}) - \widetilde{\mathbb{Q}}_T\|_{\mathrm{E}} + c\,\epsilon^{T+1}$$

and the result follows from Theorem 2.3.

Chapter 3

On Integration Methods Based on Scrambled Nets of Arbitrary Size

Abstract

We consider the problem of evaluating $I(\varphi) = \int_{[0,1)^s} \varphi(\mathbf{x})\mathrm{d}\mathbf{x}$ for a function $\varphi \in L^2[0,1)^s$. In situations where $I(\varphi)$ can be approximated by an estimate of the form $N^{-1}\sum_{n=0}^{N-1}\varphi(\mathbf{x}^n)$, with $\{\mathbf{x}^n\}_{n=0}^{N-1}$ a point set in $[0,1)^s$, it is now well known that the $\mathcal{O}_P(N^{-1/2})$ Monte Carlo convergence rate can be improved by taking for $\{\mathbf{x}^n\}_{n=0}^{N-1}$ the first $N = \lambda b^m$ points, $1 \leq \lambda < b$, of a scrambled (t,s)-sequence in base $b \geq 2$. In this paper we provide a bound for the variance of scrambled net quadrature rules which is of order $o(N^{-1})$, without any restriction on N. This bound also allows us to provide simple conditions to get an integration error of size $o_P(N^{-1/2})$ for functions that depend on the quadrature size N and, as a corollary, to establish that sequential quasi-Monte Carlo [M. Gerber and N. Chopin, 2014, *arXiv:1402.4039*] reaches the $o_P(N^{-1/2})$ convergence rate for any patterns of N. In a numerical study we show that for scrambled net quadrature rules we can relax the constraint on N without any loss of efficiency when the integrand φ is a discontinuous function while, for the univariate version of sequential quasi-Monte Carlo, taking $N = \lambda b^m$ may only provide moderate gains.

Keywords: Integration; Randomized quasi-Monte Carlo; Scrambling; Sequential quasi-Monte Carlo.

3.1 Introduction

We consider the problem of evaluating

$$I(\varphi) = \int_{[0,1)^s} \varphi(\mathbf{x})\mathrm{d}\mathbf{x}$$

for a function $\varphi \in L^2[0,1)^s$. Focussing first on unweighed quadrature rules,

$$I(P^N, \varphi) = \frac{1}{N} \sum_{n=0}^{N-1} \varphi(\mathbf{x}^n),$$

where $P^N = \{\mathbf{x}^n\}_{n=0}^{N-1}$ is a set of N points in $[0,1)^s$, the simplest way to approximate $I(\varphi)$ is to use the Monte Carlo estimator which selects for P^N a set of N independent uniform random variates on $[0,1)^s$. The central limit theorem then ensures that the variance of the approximation error $I(P^N, \varphi) - I(\varphi)$ is of order $\mathcal{O}(N^{-1})$. However, it is now well known that this rate can be improved by taking for P^N a randomized quasi-Monte Carlo (RQMC) point set. In particular, Owen (1995) proposes a randomization scheme for (t,s)-sequences in base $b \geq 2$, known as nested scrambling, such that the variance of the quadrature rule $I(P^N, \varphi)$ decreases faster than N^{-1} when P^N is the set made of the first N points of the resulting randomized sequence (Owen, 1997a, 1998). Owen (1997a, 1998) also establishes that, in this case, $\mathrm{Var}(I(P^N, \varphi)) \leq c_t N^{-1} \sigma^2$ for a constant $c_t > 0$ independent of φ and where $N^{-1}\sigma^2 = N^{-1} \int_{[0,1)^s} (\varphi(\mathbf{x}) - I(\varphi))^2 \mathrm{d}\mathbf{x}$ is the variance of a Monte Carlo quadrature rule of the same size. Interestingly, Owen (1997a) shows that the constant c_0 has the additional property to be independent of the dimension s.

In some complicated settings, the function φ can not be computed explicitly and/or the dimension s is too large for a simple unweighted quadrature rule $I(P^N, \varphi)$ to be efficient. Important examples where such a problem arise are parameter and state inference in state-space models. Recently, Gerber and Chopin (2014) have developed a sequential quasi-Monte Carlo (SQMC) algorithm to carry out sequential inference in this class of models. When this algorithm uses points taken from scrambled (t,s)-sequences as inputs, it outperforms Monte Carlo methods with an error of size $o_P(N^{-1/2})$ for continuous and bounded functions φ (Gerber and Chopin, 2014, Theorem 7).

However, all these results apply only for $N = \lambda b^m$, $1 \leq \lambda < b$, this restriction arising because (t,s)-sequences in base b are characterized by their equidistribution properties on sets of b^m consecutive points, $m \geq t$ (see Section 3.2 for a review on (t,s)-sequences). From a practical point of view, this means that a (large) variance reduction can only be obtained at the price of a sharply increasing running time, which may reduce the attractiveness of scrambled net integration methods when one is interested e.g. to reach a given level of precision at the lowest computational effort.

The objective of this paper is to study quadrature rules and SQMC based on scrambled nets of arbitrary size. Our main theoretical contribution is to provide a bound for the variance of the scrambled net quadrature rule $I(P^N, \varphi)$ which shows that the $o(N^{-1})$ convergence rate obtained by Owen (1997a, 1998) under the restriction $N = \lambda b^m$ in fact holds for any N. This bound also provides conditions to have an error of size $o_P(N^{-1/2})$ for the integral of functions φ_N which depend on the quad-

rature size N, as it typically happens in sequential estimation methods. The main consequence of this result is to establish the asymptotic superiority of SQMC over sequential Monte Carlo algorithms without any restriction of N. In addition to this bound, we show two interesting properties of scrambled net quadratures of arbitrary size. First, when points of a scrambled $(0, s)$-sequence are used, the variance of the quadrature rule admits a bound of the form $c_0^* \sigma^2 N^{-1}$ for an explicit constant $c_0^* > 0$ which is independent of the integrand φ and of the dimension s. Second, Yue and Mao (1999, Theorem 4) establish that for smooth integrands the integration error of quadratures based on scrambled sequences is of order $\mathcal{O}_P(N^{-1}(\log N)^{\frac{s-1}{2}})$. We note in this work that their computations in fact imply an error of size $\mathcal{O}_P(N^{-1})$. In a recent paper, Owen (2014) shows that this rate is the best we can achieve uniformly in N for equally weighted quadrature rules and therefore, on this class of functions, quadratures based on scrambled sequences have the optimal worst case behaviour.

The rest of this paper is organized as follows. Section 3.2 gives the notations and the background material used in this work. The announced results for quadrature rules $I(P^N, \varphi)$ based on scrambled nets are formally stated in Section 3.3. In Section 3.4 we provide conditions to get the $o_P(N^{-1/2})$ convergence rate for integrands that depend on N and discuss their application in the context of SQMC. In Section 3.5 the question of the impact of N on the convergence rate for both scrambled nets quadrature rules and for SQMC is analysed in a numerical study while Section 3.6 concludes.

3.2 Background

In this section we provide the background material on (t, s)-sequences, scrambled sequences and on the Haar-like decomposition of $L^2[0, 1)^s$ introduced by Owen (1997a). Only the concepts and the results used in this paper are presented. For a complete exposition of these notions we refer the reader, respectively, to Dick and Pillichshammer (2010, chapter 4), Owen (1995) and Owen (1997a, 1998).

For integers $s \geq 1$ and $b \geq 2$, let

$$\mathcal{E}^b = \left\{ E = \prod_{j=1}^{s} \left[a_j b^{-d_j}, (a_j + 1) b^{-d_j} \right) \subseteq [0, 1)^s,\ a_j,\ d_j \in \mathbb{N},\ a_j < b^{d_j},\ j = 1, ..., s \right\}$$

be the set of all b-ary boxes.

Let t and m be two positive integers such that $m \geq t$. Then, the point set $\{\mathbf{x}^n\}_{n=0}^{b^m-1}$ is called a (t, m, s)-net in base b if every b-ary box of volume b^{t-m} contains exactly b^t points, while the point set $\{\mathbf{x}^n\}_{n=0}^{\lambda b^m-1}$, $1 \leq \lambda < b$, is called a (λ, t, m, s)-net if every b-ary box of volume b^{t-m} contains exactly λb^t points and no b-ary box of volume b^{t-m-1} contains more than b^t points. A sequence $(\mathbf{x}^n)_{n \geq 0}$ of points in $[0, 1)^s$ is called a (t, s)-sequence in base $b \geq 2$ if, for any integers $a \geq 0$ and $m \geq t$, the

point set $\{\mathbf{x}^n\}_{n=ab^m}^{(a+1)b^m-1}$ is a (t,m,s)-net in base b. Finally, note that if $(\mathbf{x}^n)_{n\geq 0}$ is a (t,s)-sequence in base b, then, for $1\leq\lambda<b$, $\{\mathbf{x}^n\}_{n=ab^m}^{ab^m+\lambda b^m-1}$ is a (λ,t,m,s)-net for any integers $a\geq 0$ and $m\geq t$.

To introduce the Haar-like decomposition of $L^2[0,1)^s$ developed by Owen (1997a), let $u\subseteq\mathcal{S}:=\{1,...,s\}$, κ be a vector of $|u|$ non negative integers $k_{(u,j)}$, $j\in\{1,\ldots,|u|\}$, $|\kappa|=\sum_{j=1}^{|u|}k_{(u,j)}$, and

$$\mathcal{E}_{u,\kappa}^b=\left\{\prod_{j=1}^s\left[a_jb^{-d_j},(a_j+1)b^{-d_j}\right)\in\mathcal{E}^b:\ d_j=k_{(u,j)}+1 \text{ if } j\in u \text{ and } d_j=0 \text{ if } j\notin u\right\}.$$

Then, Owen (1997a) shows that

$$\varphi(\mathbf{x})=\sum_{u\subseteq\mathcal{S}}\sum_{\kappa}\nu_{u,\kappa}(\mathbf{x})$$

where, for any $u\subseteq\mathcal{S}$, $\sum_\kappa=\sum_{k_{(u,1)}=0}^{\infty}\cdots\sum_{k_{(u,|u|)}=0}^{\infty}$ and $\nu_{u,\kappa}$ is a step function, constant over each of the $b^{|u|+|\kappa|}$ sets $E\in\mathcal{E}_{u,\kappa}^b$ and which integrates to zero over any b-ary box that strictly contains a set $E\in\mathcal{E}_{u,\kappa}^b$. These step functions are mutually orthogonal and $\nu_{\varnothing,()}$ is constant over $[0,1)^s$. The resulting ANOVA decomposition of φ is given by

$$\sigma^2=\sum_{|u|>0}\sum_{\kappa}\sigma_{u,\kappa}^2 \tag{3.56}$$

with $\sigma_{u,\kappa}^2=\int_{[0,1)^s}\nu_{u,\kappa}^2(\mathbf{x})\mathrm{d}\mathbf{x}$.

Let $P^N=\{\mathbf{x}^n\}_{n=0}^{N-1}$, $\mathbf{x}^n=(x_1^n,...,x_s^n)$, be the first N points of a (t,s)-sequence in base b where, for $j=1,\ldots,s$, $x_j^n=\sum_{i=1}^{\infty}a_{jni}b^{-i}$ with $a_{jni}\in\{0,...,b-1\}$ for all n and i. Owen (1995) proposes a method to randomly permute the digits a_{jnk} such that the scrambled point set $\tilde{P}^N=\{\tilde{\mathbf{x}}^n\}_{n=0}^{N-1}$ preserves the equidistribuion properties of the original net P^N. In addition, under this randomization scheme, each $\tilde{\mathbf{x}}^n$ is marginally uniformly distributed on $[0,1)^s$ and Owen (1997a) shows that

$$\mathrm{Var}\left(I(\tilde{P}^N,\varphi)\right)=\frac{1}{N}\sum_{|u|>0}\sum_{\kappa}\Gamma_{u,\kappa}\sigma_{u,\kappa}^2 \tag{3.57}$$

where $\Gamma_{u,\kappa}$ depends on the properties of the non scrambled point set $\{\mathbf{x}^n\}_{n=0}^{N-1}$. In particular, for an arbitrary value of $N\in\mathbb{N}^*$, the gain factors $\Gamma_{u,\kappa}$ are bounded by (Hickernell and Yue, 2001, Lemma 11)

$$\Gamma_{u,\kappa}\leq b^{t+1}\left(\frac{b+1}{b-1}\right)^{s+1}. \tag{3.58}$$

When the point set P^N is a (λ,t,m,s)-net, the gain factors can be more precisely controlled. Notably, Owen (1998, Lemma 2) obtains

$$\mathrm{Var}\left(I(\tilde{P}^N,\varphi)\right)=\frac{1}{N}\sum_{|u|>0}\sum_{|\kappa|>m-t-|u|}\Gamma_{u,\kappa}\sigma_{u,\kappa}^2 \tag{3.59}$$

where $\Gamma_{u,\kappa} \leq \Gamma_t$ with $\Gamma_0 = e$ if $b \geq s$ (see (Owen, 1997b, Theorem 1) and (Hickernell and Yue, 2001, Lemma 6)) and, for $t > 0$, $\Gamma_t = b^t(b+1)^s/(b-1)^s$ (Owen, 1998, Lemma 4). Together with equation (3.59), these bounds Γ_t for the gain factors imply that

$$\mathrm{Var}\left(I(\tilde{P}^N, \varphi)\right) = o(N^{-1}), \quad \mathrm{Var}\left(I(\tilde{P}^N, \varphi)\right) \leq \Gamma_t \frac{\sigma^2}{N} \tag{3.60}$$

where we recall that $\tilde{P}^N$ contains the fist $N = \lambda b^m$ points of a scrambled (t, s)-sequence in base b.

We conclude this section by noting that all the results presented in this work also hold for the computationally cheaper scrambling method proposed by Matoŭsek (1998), although in what follows we will only refer to the scrambling technique developed by Owen (1995) for ease of presentation. In addition, even if it is not always explicitly mentioned, all the scrambled nets we consider in this work are made of the first N points of a scrambled (t, s)-sequence.

3.3 Quadratures based on scrambled nets of arbitrary size

3.3.1 Error bounds

A first result concerning the error bound of quadratures based on scrambled nets of an arbitrary size N can be directly deduced from (3.57) and (3.58). Indeed, if $\tilde{P}^N$ contains the first $N \in \mathbb{N}^*$ points of a scrambled (t, s)-sequence in base $b \geq 2$, these two bounds imply that

$$\mathrm{Var}\left(I(\tilde{P}^N, \varphi)\right) \leq \frac{\sigma^2}{N} b^{t+1} \left(\frac{b+1}{b-1}\right)^{s+1} \tag{3.61}$$

so that the variance of scrambled nets quadrature is never larger than a constant time the Monte Carlo variance.

The following Theorem is the main result of this work and provides a sharper bound for the integration error (see A for a proof).

Theorem 3.1. *Let* $\varphi \in L^2[0,1)^s$, $\sigma^2 = \int_{[0,1)^s} \varphi^2(\mathbf{x})\mathrm{d}\mathbf{x} - \left(\int_{[0,1)^s} \varphi(\mathbf{x})\mathrm{d}\mathbf{x}\right)^2$ *and* $\tilde{P}^N = \{\tilde{\mathbf{x}}^n\}_{n=0}^{N-1}$ *be the first* N *points of a* (t, s)*-sequence in base* $b \geq 2$ *scrambled as in Owen*

(1995). Let $N \in \mathbb{N}^*$ be such that $b^k \leq N < b^{k+1}$ for an integer $k \geq t+s+1$. Then,

$$\mathrm{Var}\left(\frac{1}{N}\sum_{n=0}^{N-1}\varphi(\tilde{\mathbf{x}}^n)\right) \leq b^t\left(\frac{b+1}{b-1}\right)^s\frac{2}{N}\Bigg\{(1+c_b)B_t^{(k)} + c_b\left[B_{t+1}^{(k)} + \sum_{|u|>0}\frac{1}{b^{\frac{k-1-t-|u|}{2}}}\sum_{|\kappa|\leq k-1-t-|u|} b^{\frac{|\kappa|}{2}}\sigma_{u,\kappa}^2\right] + \sigma^2\frac{b^{t+1}(b+1)}{N(b-1)}\Bigg\}$$

where $c_b = \frac{(b-1)^{1/2}}{b^{1/2}-1}$ and, for $c \in \{0,\ldots,k-s-1\}$,

$$B_c^{(k)} = \sum_{|u|>0}\sum_{|\kappa|>k-c-|u|}\sigma_{u,\kappa}^2 + \sum_{|u|>0}\frac{1}{b^{k-c-|u|}}\sum_{|\kappa|\leq k-c-|u|}\sigma_{u,\kappa}^2 b^{|\kappa|}.$$

Thanks to Kronecker's Lemma, this Theorem implies that for any square integrable function the error is of size $o_P(N^{-1/2})$ without any restriction on N. Due to its importance for this work, Kronecker's Lemma is recalled in Lemma 3.1 below (see e.g. Shiryaev, 1996, Lemma 2, p.390, for a proof).

Lemma 3.1 (Kronecker's Lemma)**.** *Let $(d_n)_{n\geq 1}$ be a sequence of positive increasing numbers such that $d_n \to +\infty$ as $n \to +\infty$, and let $(z_n)_{n\geq 1}$ be a sequence of numbers such that $\sum_{n=1}^{+\infty} z_n < +\infty$. Then, as $n \to +\infty$,*

$$\frac{1}{d_n}\sum_{i=1}^{n} d_i z_i \to 0.$$

When $t = 0$, we note from the proof of Theorem 3.1 that the variance of quadratures based on points taken from a scrambled $(0,s)$-sequences is never larger than a universal constant c_0^* time the Monte Carlo variance. These two results are collected in the following Corollary.

Corollary 3.1. *Consider the set-up of Theorem 3.1. Then, for any $\varphi \in L^2[0,1)^s$, we have*

$$\mathrm{Var}\left(\frac{1}{N}\sum_{n=0}^{N-1}\varphi(\tilde{\mathbf{x}}^n)\right) = o(N^{-1}).$$

In addition, for $t = 0$,

$$\mathrm{Var}\left(\frac{1}{N}\sum_{n=0}^{N-1}\varphi(\tilde{\mathbf{x}}^n)\right) \leq \frac{\sigma^2}{N}e\,(3+2\sqrt{2}) \approx 15.84\frac{\sigma^2}{N}.$$

Proof. To prove the error rate, let $\tilde{\sigma}^2_{u,l} = \sum_{\kappa:|\kappa|=l} \sigma^2_{u,\kappa}$ for $l \in \mathbb{N}$ and note that, for any fixed integers $a > 0$, $0 \leq c < k - s$ and $u \subseteq \mathcal{S}$,

$$\begin{aligned}\frac{1}{b^{a(k-c-|u|)}} \sum_{|\kappa| \leq k-c-|u|} \sigma^2_{u,\kappa} b^{a|\kappa|} &= \frac{1}{b^{a(k-c-|u|)}} \sum_{l=0}^{k-c-|u|} b^{al}\, \tilde{\sigma}^2_{u,l} \\ &= \frac{1}{b^{a(k-c-|u|+1)}} \sum_{l=1}^{k-c-|u|+1} b^{al}\, \tilde{\sigma}^2_{u,l-1}\end{aligned}$$

which converges to zero by Kronecker's Lemma. Also, because $\sum_{|u|>0} \sum_{\kappa} \sigma^2_{u,\kappa} = \sigma^2$, this shows that, as $N \to +\infty$, $B^{(k)}_t \to 0$ and $B^{(k)}_{t+1} \to 0$ and therefore, using Theorem 3.1,

$$N\mathrm{Var}\left(\frac{1}{N}\sum_{n=0}^{N-1} \varphi(\tilde{\mathbf{x}}^n)\right) \to 0$$

as $N \to +\infty$. The proof of the bound for $t = 0$ is postponed to B. □

At this point it worth mentioning that the $o_P(N^{-1/2})$ convergence rate for quadratures based on scrambled nets of arbitrary size was simultaneously established by Art B. Owen (personal communication) using a more direct proof. Nevertheless, the bound given in Theorem 3.1 also allows to study situations where the integrand depends on the size of the quadrature rule N, as explained in Section 3.4.

3.3.2 Error rate for smooth integrands

For a hyperrectangle $J = [\boldsymbol{a}, \boldsymbol{b}] \subset [0,1)^s$ and a set $u \subseteq \mathcal{S}$, let $J^u = [\boldsymbol{a}^u, \boldsymbol{b}^u]$ where we write $\mathbf{x}^u$ the projection of $\mathbf{x} \in [0,1)^s$ onto $[0,1)^u$, the $|u|$-dimensional unit hypercube with coordinates in u, and

$$\Delta_u(\varphi, J) = \sum_{v \subseteq u} (-1)^{|v|} \varphi_v(\boldsymbol{a})$$

where $\varphi_v(\boldsymbol{a}) = \varphi(\mathbf{x})$ with $x_i = a_i$ if $i \in v$ and $x_i = b_i$ otherwise.

Yue and Mao (1999) analyse the integration error for the class of real valued functions φ that satisfy the following general Lipschitz condition:

$$|\Delta_u(\varphi, J)| \leq C\lambda_u(J^u), \quad \forall u \subseteq \mathcal{S}, \quad \forall J = [\boldsymbol{a}, \boldsymbol{b}] \subset [0,1)^s \tag{3.62}$$

for a constant $C > 0$ and where λ_u is the Lebesgue measure on $[0,1)^u$. For these smooth integrands, Yue and Mao (1999) establish that

$$\sigma^2_{u,\kappa} \leq C^2 b^{-2|\kappa|} \left(\frac{2b^2 - 3b + 1}{b^2}\right)^{|u|}$$

and therefore, according to Owen (1998, Theorem 2), we have, for $m \geq t+s-1$,

$$\sum_{|u|>0} \sum_{|\kappa|>m-t-|u|} \sigma_{u,\kappa}^2 = \mathcal{O}\left(b^{-2m} m^{s-1}\right) \tag{3.63}$$

showing that the error is of size $\mathcal{O}_P(N^{-1.5}(\log N)^{\frac{s-1}{2}})$ for quadratures based on scrambled (λ, t, m, s)-nets. From this results, Yue and Mao (1999, Theorem 4) deduce that quadratures based on nets of arbitrary size have an error rate of order $\mathcal{O}_P(N^{-1}(\log N)^{\frac{s-1}{2}})$ but as we will see in the next few lines the right rate is in fact $\mathcal{O}_P(N^{-1})$.

As previously, $\tilde{P}^N = \{\tilde{\mathbf{x}}^n\}_{n=0}^{N-1}$ denotes the set containing the first $b^{k+1} > N \geq b^k$ points of a scrambled (t, s)-sequence in base b. The standard way to analyse the variance of a scrambled net quadrature rule of arbitrary size is to decompose $\tilde{P}^N$ into scrambled (a_m, t, m, s)-nets $\tilde{P}_m$, $m = t, ..., (k-t+1)$, and a remaining set $\tilde{P}$ that contains $\tilde{n} < b^t$ points (see the proof of Theorem 3.1 for more details). Let $\tilde{P}' = \tilde{P} \cup_{m=t}^{t+s-2} \tilde{P}_m$. Then, using trivial inequalities, we have

$$\mathrm{Var}\left(I(\tilde{P}^N, \varphi)\right) \leq \frac{1}{N^2} \left(\mathrm{Var}\left(\sum_{n \in \tilde{P}'} \varphi(\tilde{\mathbf{x}}^n) \right)^{1/2} + \sum_{m=t+s-1}^{k} \mathrm{Var}\left(\sum_{n \in \tilde{P}_m} \varphi(\tilde{\mathbf{x}}^n) \right)^{1/2} \right)^2.$$

From (3.61), $\mathrm{Var}\left(\sum_{n \in \tilde{P}'} \varphi(\tilde{\mathbf{x}}^n)\right)^{1/2} < c_1$ for a constant c_1 while, using (3.63),

$$\sum_{m=t+s-1}^{k} \mathrm{Var}\left(\sum_{n \in \tilde{P}_m} \varphi(\tilde{\mathbf{x}}^n) \right)^{1/2} = \mathcal{O}\left(\sum_{m=t+s-1}^{k} b^{-m/2} m^{\frac{s-1}{2}} \right) = \mathcal{O}(1)$$

since $\sum_{m=t+s-1}^{\infty} b^{-m/2} m^{\frac{s-1}{2}} < +\infty$. We therefore conclude that $N^2 \mathrm{Var}\left(I(\tilde{P}^N, \varphi)\right) < \bar{c}$ for N large enough and for a constant $\bar{c}$. Recently, Owen (2014, Theorem 2) has shown that the best possible error rate we can have uniformly on N is of order $\mathcal{O}_P(N^{-1})$ and therefore there exists a constant $\underline{c} < \bar{c}$ such that, for N large enough,

$$\underline{c} < N^2 \mathrm{Var}\left(I(\tilde{P}^N, \varphi)\right) < \bar{c}.$$

Hence, on the class of function satisfying the general Lipschitz condition (3.62), scrambled net quadrature rules have the optimal worst case behaviour.

3.4 Error rate for integrands that depend on the quadrature size

We now analyse the behaviour of the quadrature $I(\tilde{P}^N, \varphi_N)$ where $(\varphi_N)_{N \geq 1}$ is a sequence of real valued functions. In practice, the sequence of functions $(\varphi_N)_{N \geq 1}$ is

often such that, as $N \to +\infty$, $\varphi_N \to \varphi$ where $I(\varphi)$ is the quantity of interest. The classical situation where this set-up occurs is when we are estimating $I(\varphi)$ using a sequential method such as the array-RQMC algorithm developed by L'Ecuyer et al. (2006) or the SQMC algorithm proposed by Gerber and Chopin (2014).

Using Theorem 3.1, we can deduce the following result concerning the error size of the quadrature rule $I(\tilde{P}^N, \varphi_N)$.

Corollary 3.1. *Consider the set-up of Theorem 3.1. Let $(\varphi_N)_{N\geq 1}$ be a sequence of functions such that, $\forall N \in \mathbb{N}^*$, $\varphi_N \in L^2[0,1)^s$, and let*

$$\sigma_N^2 = \int_{[0,1)^s} \left(\varphi_N(\mathbf{x}) - \int_{[0,1)^s} \varphi_N(\mathbf{v}) \mathrm{d}\mathbf{v} \right)^2 \mathrm{d}\mathbf{x}.$$

Assume that, for any $u \subseteq \{1, \ldots, s\}$ and for any $\kappa(u)$, we have, as $N \to +\infty$,

$$\sigma_N^2 \to \sigma^2 < +\infty, \quad \sigma_{N,u,\kappa}^2 \to \sigma_{u,\kappa}^2,$$

where $\sigma_N^2 = \sum_{|u|>0} \sum_{\kappa} \sigma_{N,u,\kappa}^2$ and $\sigma^2 = \sum_{|u|>0} \sum_{\kappa} \sigma_{u,\kappa}^2$. Then,

$$\mathrm{Var}\left(\frac{1}{N} \sum_{n=0}^{N-1} \varphi_N(\tilde{\mathbf{x}}^n) \right) = o(N^{-1}).$$

Proof. Let k be the largest power of b such that $b^k \leq N$. Then, by Theorem 3.1, to prove the result we first need to show that, for $a \in \{\frac{1}{2}, 1\}$ and $c \in \{t, t+1\}$, we have

$$\sum_{|u|>0} \frac{1}{b^{a(k-c-|u|)}} \sum_{|\kappa| \leq k-c-|u|} \sigma_{N,u,\kappa}^2 b^{a|\kappa|} = o(1).$$

To establish this result, let a and c be as above, $k' = k - c - |u| + 1$ (for k large enough), $\tilde{k} = \lfloor k'/2 \rfloor$ and $S_{u,p}^N = \sum_{l=1}^{p+1} \tilde{\sigma}_{N,u,l-1}^2$ where $\tilde{\sigma}_{N,u,l}^2$ is defined as in the proof of Corollary 3.1. Note that the positive and increasing sequence $(S_{u,p}^N)_{p\geq 1}$ converges to $\sigma_{N,u}^2 = \sum_{|\kappa|>0} \sigma_{N,u,\kappa}^2$ as $p \to +\infty$. Then, using summation by part and similar computations as in the proof of Kronecker's Lemma (see e.g. Shiryaev, 1996, Lemma 2, p.390), we have

$$\begin{aligned}
\frac{1}{b^{a(k-c-|u|)}} \sum_{l=0}^{k-c-|u|} \tilde{\sigma}^2_{N,u,l} b^{al} &= \frac{1}{b^{ak'}} \sum_{l=1}^{k'} \tilde{\sigma}^2_{N,u,l-1} b^{al} \\
&= S^N_{u,k'} - \frac{1}{b^{ak'}} \sum_{l=1}^{k'-1} (b^{a(l+1)} - b^{al}) S^N_{u,l} \\
&= S^N_{u,k'} - \sum_{l=1}^{\tilde{k}-1} \frac{b^{a(l+1)} - b^{al}}{b^{ak'}} S^N_{u,l} - \sum_{l=\tilde{k}}^{k'-1} \frac{b^{a(l+1)} - b^{al}}{b^{ak'}} \sigma^2_{N,u} \\
&- \frac{1}{b^{ak'}} \sum_{l=\tilde{k}}^{k'-1} (b^{a(l+1)} - b^{al})(S^N_{u,l} - \sigma^2_{N,u}) \\
&\leq \frac{b^{a\tilde{k}}}{b^{ak'}} \sigma^2_{N,u} + (\sigma^2_{N,u} - S^N_{u,\tilde{k}})
\end{aligned}$$

so that

$$\sum_{|u|>0} \frac{1}{b^{a(k-c-|u|)}} \sum_{|\kappa| \leq k-c-|u|} \sigma^2_{N,u,\kappa} b^{a|\kappa|} \leq \sum_{|u|>0} b^{a(\tilde{k}-k')} \sigma^2_{N,u} + \left(\sigma^2_N - \sum_{|u|>0} S^N_{u,\tilde{k}} \right). \quad (3.64)$$

Then, using Fatou's Lemma,

$$\begin{aligned}
0 \leq \limsup_{k \to +\infty} \left(\sigma^2_N - \sum_{|u|>0} S^N_{u,\tilde{k}} \right) &= \limsup_{k \to +\infty} \left(\sigma^2_N - \sum_{|u|>0} \sum_{l \geq 0} \mathbb{I}(l \leq \tilde{k}) \tilde{\sigma}^2_{N,u,l} \right) \\
&\leq \sigma^2 - \liminf_{k \to +\infty} \sum_{|u|>0} \sum_{l \geq 0} \mathbb{I}(l \leq \tilde{k}) \tilde{\sigma}^2_{N,u,l} \\
&\leq \sigma^2 - \sum_{|u|>0} \sum_{l \geq 0} \liminf_{k \to +\infty} \mathbb{I}(l \leq \tilde{k}) \tilde{\sigma}^2_{N,u,l} \\
&= 0
\end{aligned}$$

because each $\tilde{\sigma}^2_{N,u,l}$ is a finite sum of some $\sigma^2_{N,u,\kappa}$'s and, by assumption, $\sigma^2_{N,u,\kappa} \to \sigma^2_{u,\kappa}$ for any u and κ. This shows that the second term of (3.64) converges to zero as $N \to +\infty$. The above computations also show that, for any $u \subseteq \mathcal{S}$, $\sigma^2_{N,u}$ converges to $\sum_{|\kappa|>0} \sigma^2_{u,\kappa}$ so that $b^{a(\tilde{k}-k')} \sigma^2_{N,u} \to 0$ as $N \to +\infty$. Hence, the right-hand side of (3.64) goes to zero as N increases, as required. To conclude the proof note that these computations also imply that, as $N \to +\infty$,

$$\sum_{|u|>0} \sum_{|\kappa| \leq k-c-|u|} \sigma^2_{N,u,\kappa} \to 0.$$

□

A direct consequence this Corollary 3.1 is to relax the constraint on N in Gerber and Chopin (2014, Theorem 7), showing that on the class of continuous and bounded functions SQMC asymptotically outperforms standard sequential Monte Carlo algorithms without any restriction on how the number of "particles" N grows.

Providing a complete description of SQMC is behind the scope of this work (see Section 3.5.2 for an example of SQMC algorithm). Nevertheless, to get some insight about how Corollary 3.1 applies to this class of methods, we illustrate this results by studying a scrambled net version of the sampling importance resampling (SIR) algorithm proposed by Rubin (1988), which is iteratively used in SQMC.

To keep the presentation simple we consider a (toy) SIR algorithm designed to estimate the univariate expectation $\pi(f) := \int_{[0,1)} f(x)\pi(x)\mathrm{d}x$, with π a density function on $[0,1)$. Let $q(x)\mathrm{d}x$ be a proposal distribution on the same space, $P_1^N = \{x_1^n\}_{n=0}^{N-1}$ be a (deterministic) QMC point set in $[0,1)$ and $\tilde{P}_2^N = \{\tilde{x}_2^n\}_{n=0}^{N-1}$ be a scrambled net. Then, noting F_μ^{-1} the (generalized) inverse of F_μ, the CDF corresponding to the probability measure μ on $\mathbb{R}$, one QMC version of the SIR algorithm may be as follows:

1. Compute $z_1^n = F_q^{-1}(x_1^n)$ and $w^n = \pi(z_1^n)/q(z_1^n)$ for $n = 1, \ldots, N$;

2. Compute $I(\tilde{P}_2^N, \varphi_N)$ where $\varphi_N = f \circ F_N^{-1}$ with F_N^{-1} the (generalized) inverse of the empirical CDF $F_N(z) = \sum_{n=1}^N \frac{w^n}{\sum_{m=1}^N w^m} \mathbb{I}(z_1^n \leq x)$.

Assume that the functions $f(z)$ and $\pi(z)/q(z)$ are continuous and bounded and that F_q^{-1} is continuous. Then, Gerber and Chopin (2014, Theorem 1) shows that $\varphi_N \to \varphi = f \circ F_\pi^{-1}$, with $I(\varphi) = \pi(f)$ the quantity we want to estimate. In addition, it can be shown that, under these assumptions, step 2. of the above SIR algorithm verifies the assumptions of Corollary 3.1 (see the proof of (Gerber and Chopin, 2014, Theorem 7)) so that the quadrature rule $I(\tilde{P}_2^N, \varphi_N)$ reaches, without any constraint on N, the $o_P(N^{-1/2})$ convergence rate. Note that for sake of simplicity we assume here that P_1^N is a deterministic QMC point set but this analysis extends trivially to the case where we also use a scrambled net in step 1. of this QMC SIR algorithm.

3.5 Numerical Study

In this section we illustrate the main findings of this paper. All the simulations rely on a Sobol' sequence that is scrambled using the method proposed by Owen (1995). We recall that $b = 2$ for the Sobol' sequence. All means square errors (MSEs) presented below are estimated from 100 independent repetitions.

3.5.1 Scrambled net quadratures

As in He and Owen (2014), our objective is to estimate the s-dimensional integral $I(\varphi_i)$, $i = 1, \ldots, 3$, where

$$\varphi_1(\mathbf{x}) = \sum_{i=1}^{s} x_i, \quad \varphi_2(\mathbf{x}) = \max\left(\sum_{i=1}^{s} x_i - \frac{s}{2}, 0\right), \quad \varphi_3(\mathbf{x}) = \mathbb{I}_{\left(\sum_{i=1}^{s} x_i > \frac{s}{2}\right)}(\mathbf{x}).$$

Note that the integrands φ_1 and φ_2 are both Lipschitz continuous but φ_2 is not everywhere differentiable. For $i \in \{1, 2, 3\}$, we estimate the integral $I(\varphi_i)$ using the quadrature rule $I(\tilde{P}^N, \varphi_i)$ where, as mentioned above, $\tilde{P}^N$ is the set containing the first N points of a scrambled Sobol' sequence.

Figure 3.1 shows the evolution of the MSEs as a function of N for the quadrature rules $I(\tilde{P}^N, \varphi_i)$, $i = 1, \ldots, 3$. Results are presented for N ranging from 1 to 2^{16} and for $s = 3$. In addition to the MSEs we have reported the Monte Carlo $\mathcal{O}(N^{-1})$ reference line to illustrate the result of Corollary 3.1, namely that the convergence rate is faster than N^{-1} for any pattern of N. To compare quadrature rules based on nets of arbitrary size with those based on (λ, t, m, s)-nets, Figure 3.1 also shows the evolution of the MSEs along the subsequence $N = 2^m$. The interesting point to note here is that the advantage of using (λ, t, m, s)-nets over nets of arbitrary size decreases as the integrand becomes "less smooth". Indeed, for the everywhere differentiable and Lipschitz function φ_1 it is clear from Figure 3.1 that there is no gain to take $N \neq 2^m$ since we can observe that the cheapest way to reach any given level of MSE is to select for N a powers 2. For the function φ_2 the same observation hold only for $N \geq 2^5$ and the gain of using (λ, t, m, s)-nets is clearly smaller than for the estimation of $I(\varphi_1)$. Finally, the advantage of taking a powers of 2 for the quadrature size has completely disappeared for the discontinuous function φ_3.

To understand these observations recall that the variance of the quadrature rule $I(\tilde{P}^N, \varphi)$ is bounded above by (see Section 3.3.2)

$$\mathrm{Var}\left(I(\tilde{P}^N, \varphi)\right) \leq \frac{C}{N^2}\left(\mathbb{I}(N = 2^k) + \sum_{j=t+s-1}^{k} \mathrm{Var}\left(\sum_{n \in \tilde{P}_j} \varphi(\tilde{\mathbf{x}}^n)\right)^{1/2}\right)^2 \tag{3.65}$$

for a constant C and where, in our setting, the $\tilde{P}_j$'s are scrambled (t, j, s)-nets in base $b = 2$ and k is the largest integer such that $2^k \leq N$. In addition, note that the cost of choosing an arbitrary value for N is to impose a lower bound of order N^{-2} for the variance of the quadrature rule since it is the best rate we can achieve uniformly on N (Owen, 2014, Theorem 2). Therefore, together with inequality (3.65), this shows that $\mathrm{Var}(I(\tilde{P}^N, \varphi)) = \mathcal{O}(N^{-2})$ for integrands φ which are such that $\mathrm{Var}(I(\tilde{P}^{\lambda b^m}, \varphi)) = \mathcal{O}(b^{-\alpha m})$ for a $\alpha \geq 2$. On the contrary, for a non smooth integrand φ which verifies $\mathrm{Var}(I(\varphi, \tilde{P}^{\lambda b^m})) = \mathcal{O}(b^{-\alpha m})$ for a $\alpha \in (0, 2)$, the upper

bound (3.65) suggests that we will obtain the same convergence rate regardless of the pattern for N.

As illustrated in Figure 3.1, the error size of quadratures based on scrambled (λ, t, m, s)-nets depends positively on the smoothness of the integrand (for theoretical results, see Owen, 1997b, 1998; Yue and Mao, 1999; Hickernell and Yue, 2001). Hence, taking $N = \lambda b^k$ is the best choice the integrands φ_1 and φ_2 since then the MSE goes to zero much faster than N^{-2}. Note that for φ_2 the MSE obtained by taking $N = \lambda 2^k$ decreases slower than for φ_1 so that, as a result, N should be larger to rule out the choice $N \neq \lambda b^k$. Finally, for the discontinuous function φ_3 the convergence rate of the MSE when using (λ, t, m, s)-nets is too slow for the choice of N to influence that of the MSE.

3.5.2 Likelihood function estimation in state-space models

We now study the problem of estimating the likelihood function of the following generic univariate state-space model

$$\begin{cases} y_k | z_k \sim \mathcal{N}\left(\mu_y(z_k), \sigma_y^2(z_k)\right), & k \geq 0 \\ z_k | z_{k-1} \sim \mathcal{N}\left(\mu_z(z_{k-1}), \sigma_z^2(z_{k-1})\right), & k \geq 1 \\ z_0 \sim \mathcal{N}(\mu_0, \sigma_0^2) \end{cases} \tag{3.66}$$

where $(y_k)_{k\geq 0}$ is the observation process, $(z_k)_{k\geq 0}$ is the hidden Markov process and where $\mu_q : \mathbb{R} \to \mathbb{R}$ and $\sigma_q : \mathbb{R} \to \mathbb{R}^+$, $q \in \{z, y\}$, are known functions.

Given a set of T observations $\{y_k\}_{k=0}^{T-1}$ we denote by $p(y_{0:T-1})$ the likelihood function of the model defined by (3.66), which can not be computed explicitly. Indeed, writing $f(\cdot, \mu, \sigma^2)$ the density function of the $\mathcal{N}(\mu, \sigma^2)$ distribution, it is easy to see that $p(y_{0:T-1}) = I(\varphi_T)$ where $\varphi_T : [0,1)^T \to \mathbb{R}$ is given by

$$\varphi_T(x_0, \ldots, x_{T-1}) = \tilde{\varphi}_T \circ F_T^{-1}(x_0, \ldots, x_{T-1})$$

with $\tilde{\varphi}_T(z_0, \ldots, z_{T-1}) = \prod_{k=0}^{T-1} f(y_k, \mu_y(z_k), \sigma_y^2(z_k))$ and F_T the Rosenblatt transformation (see Rosenblatt, 1952, for a definition) of the probability measure

$$f(z_0, \mu_0, \sigma_0^2)\mathrm{d}z_0 \prod_{k=1}^{T-1} f(z_k, m_z(z_{k-1}), \sigma_z^2(z_{k-1}))\mathrm{d}z_k.$$

In practical scenarios, the time horizon T is large (at least several dozen) and the function φ_T is concentrated in a tiny region of the integration domain. Consequently, simple unweighed quadrature rules require a huge amount of points to provide a precise estimate of $p(y_{0:T-1})$. An efficient way to get an unbiased estimate $p^N(y_{0:T-1})$ of $p(y_{0:T-1})$ is to use a SQMC algorithm (Gerber and Chopin, 2014), that is a QMC version of sequential Monte Carlo methods which are now standard tools to handle

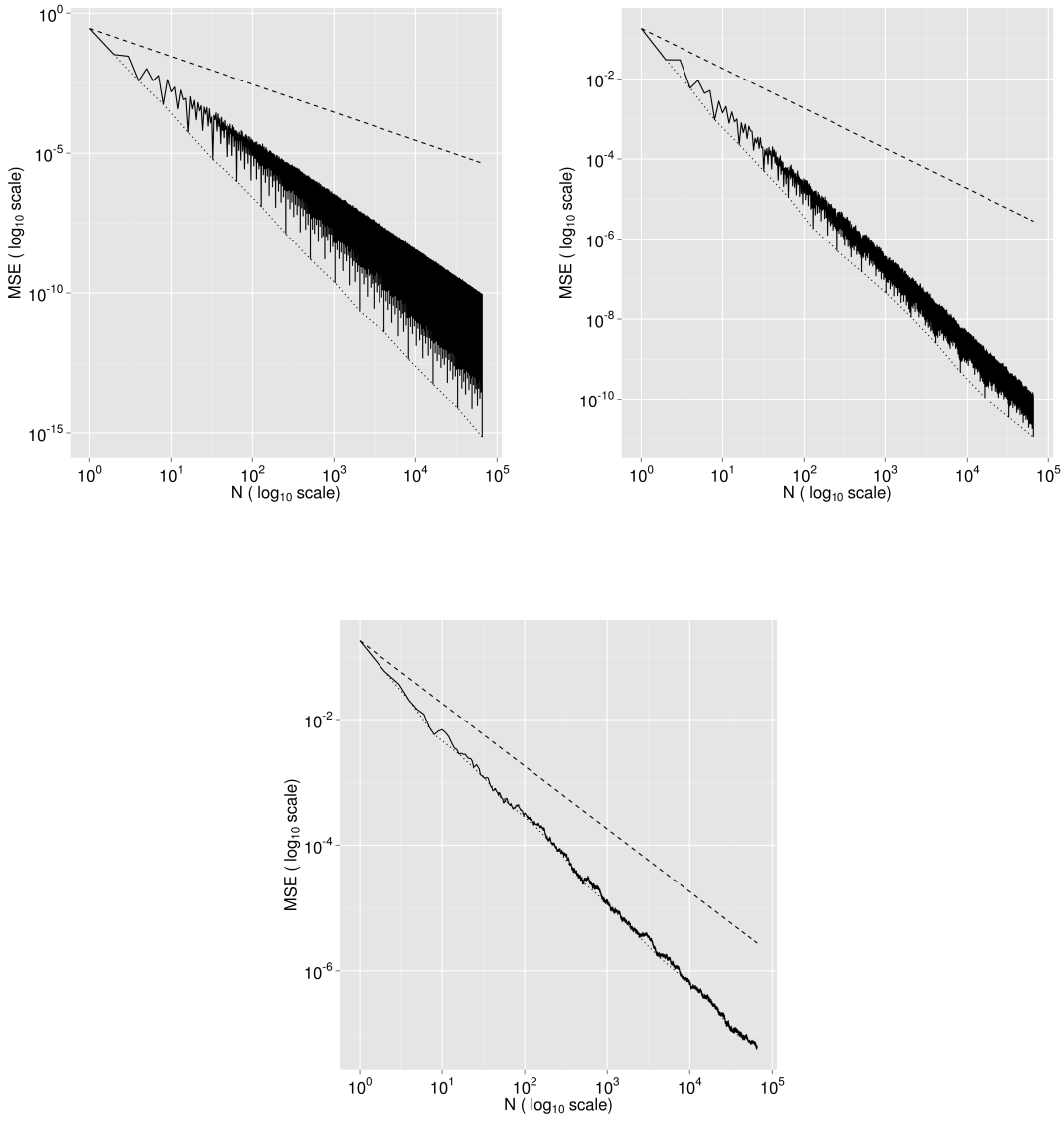

Figure 3.1: Mean square error of $I(\tilde{P}^N, \varphi_1)$ (top-left), $I(\tilde{P}^N, \varphi_2)$ (top-right) and $I(\tilde{P}^N, \varphi_3)$ where $\tilde{P}^N$ contains the first N points of a scrambled Sobol' sequence. The dashed lines are the $\mathcal{O}(N^{-1})$ Monte Carlo reference lines, the dotted lines present the results along the subsequence $N = 2^m$ for $m = 0, \ldots, 16$ and the solid lines the MSEs for any $N \in \{1, \ldots 2^{16}\}$. The results are obtained from 100 independent repetitions.

Algorithm 3.1 SQMC Algorithm to estimate $p(y_{0:T-1})$ in the state-space model (3.66)

1: Generate a RQMC point set $\{\tilde{x}_0^n\}_{n=1}^N$ in $[0,1)$.
2: **for** $n = 1 \to N$ **do**
3: Compute $z_0^n = \mu_0 + \sigma_0 \Phi^{-1}(\tilde{x}_0^n)$ and $w_0^n = f\left(y_0; \mu_y(z_0^n), \sigma_y^2(z_0^n)\right)$.
4: **end for**
5: **for** $n = 1 \to N$ **do**
6: Normalize the weights: $W_0^n = w_0^n / \sum_{m=1}^N w_0^m$.
7: **end for**
8: Compute $p^N(y_0) = N^{-1} \sum_{n=1}^N w_0^n$.
9: **for** $k = 1 \to T-1$ **do**
10: Generate a RQMC point set $\{\tilde{\mathbf{x}}_k^n\}_{n=1}^N$ in $[0,1)^2$; let $\tilde{\mathbf{x}}_k^n = (\tilde{x}_k^n, \tilde{v}_k^n)$.
11: **for** $n = 1 \to N$ **do**
12: Compute $\tilde{z}_{k-1}^n = F_{N,k-1}^{-1}(\tilde{x}_k^n)$ where $F_{N,k-1}(z) = \sum_{m=0}^N W_{k-1}^m \mathbb{I}(z_{k-1}^m \leq z)$.
13: Compute $z_k^n = \mu_z(\tilde{z}_{k-1}^n) + \sigma_z(\tilde{z}_{k-1}^n)\Phi^{-1}(\tilde{v}_k^n)$.
14: Compute $w_k^n = f\left(y_k; \mu_y(z_k^n), \sigma_y^2(z_k^n)\right)$.
15: **end for**
16: **for** $n = 1 \to N$ **do**
17: Normalize the weights: $W_k^n = w_k^n / \sum_{m=1}^N w_k^m$.
18: **end for**
19: Compute $p^N(y_{0:k}) = p^N(y_{0:k-1})\, N^{-1} \sum_{n=1}^N w_k^n$.
20: **end for**
21: **return** $p^N(y_{0:T-1})$.

this kind of problems (see e.g. Doucet et al., 2001). The suitable SQMC algorithm for the generic state-space model (3.66) is presented in Algorithm 3.1, where we use the standard notation $\Phi(\cdot)$ for the CDF of the $\mathcal{N}(0,1)$ distribution.

In this simulation study we analyse the MSE of $\log p^N(y_{0:T-1})$ when at steps 1 and 10 of Algorithm 3.1 the RQMC point sets are the first N points of independent scrambled Sobol' sequences, where $N = 4i$ for $i = 3, \ldots, 2^{11}$. Note that, in Algorithm 3.1, we have $\sum_{n=1}^N w_k^n = \sum_{n=1}^N \varphi_{N,k}(\tilde{\mathbf{x}}_k^n)$ where, for $\mathbf{x} = (x_1, x_2) \in [0,1)^2$,

$$\varphi_{N,k}(\mathbf{x}) = f\left(y_k, \mu_y \circ g(\mathbf{x}), \sigma_y^2 \circ g(\mathbf{x})\right), \quad g(\mathbf{x}) = \mu_z \circ F_{N,k-1}^{-1}(x_1) + \sigma_z \circ F_{N,k-1}^{-1}(x_1)\Phi^{-1}(x_2).$$

Since the function $F_{N,k-1}^{-1}$ is discontinuous, the results of the previous subsection therefore suggest that the gain of restricting N to be powers of the Sobol' sequence is small in the context of SQMC. In addition, it is wroth remarking that this gain will also depend on the regularity of the functions μ_q and σ_q, $q \in \{y, z\}$.

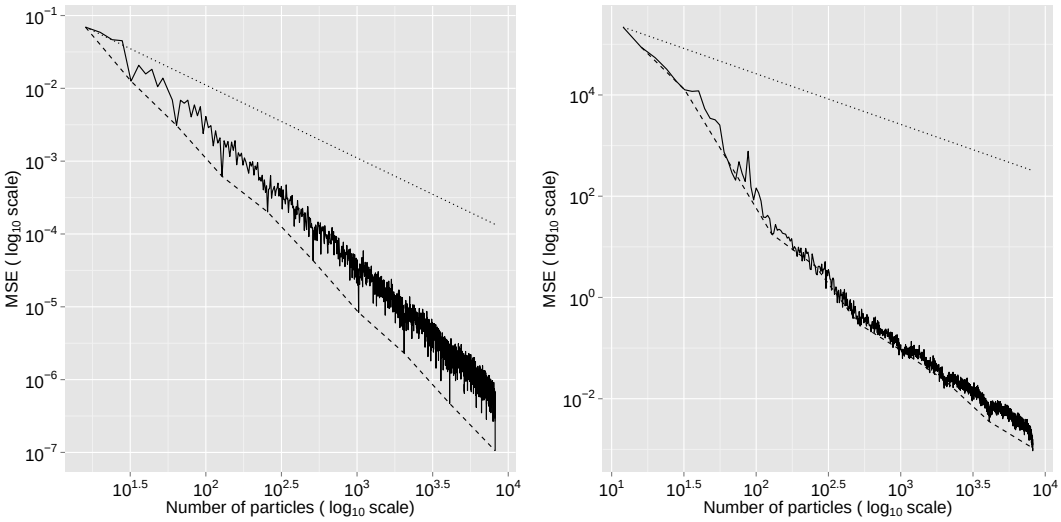

Figure 3.2: Mean square error for the estimation of $\log p(y_{0:T-1})$ in the SV model (3.67) (left plot) and in the toy example (3.68) (right plot). The dotted lines are Monte Carlo $\mathcal{O}(N^{-1})$ reference lines, the dashed lines present the results for SQMC for $N = 2^m$, $m = 3, \ldots, 13$, while the solid lines are for SQMC with $N = 4i$, $i = 3, \ldots, 2^{11}$. The results are obtained from 100 independent runs of Algorithm 3.1.

Stochastic volatility (SV) model. We first consider the following simple univariate SV model

$$\begin{cases} y_k | z_k \sim \mathcal{N}\left(0, e^{z_k}\right), & k \geq 0 \\ z_k | z_{k-1} \sim \mathcal{N}\left(0.9 z_{k-1}, 0.1\right), & k \geq 1 \\ z_0 \sim \mathcal{N}(0, \frac{0.1}{1-0.9^2}) \end{cases} \tag{3.67}$$

from which a set of 100 observations is generated. Figure 3.2 (left plot) presents the MSE of the estimator $p^N(y_{0:T-1})$ and the $\mathcal{O}(N^{-1})$ Monte Carlo reference line. As expected, we see that the $o_P(N^{-1})$ convergence rate for the SQMC algorithm holds uniformly on N. However, we observe in this example that selecting $N = 2^m$ is optimal as soon as $N \geq 2^7$ in the sense that this choice guaranties the smallest MSE for a given computational budget. The fact that very quickly it is desirable to restrict N to be a power of 2 is not surprising because the SV model (3.67) is an example of state-space model (3.66) where the functions μ_q and σ_q^2, $q \in \{y, z\}$, are very smooth.

A non-linear and non-stationary model We now consider the following non-linear and non-stationary well known toy example in the particle filtering literature

(see e.g. Gordon et al., 1993)

$$\begin{cases} y_k|z_k \sim \mathcal{N}\left(\frac{z_k^2}{20}, 1\right), & k \geq 0 \\ z_k|z_{k-1} \sim \mathcal{N}\left(0.5 z_{k-1} + 25\frac{z_{k-1}}{1+z_{k-1}^2} + 8\cos(1.2k), 10\right), & k \geq 1 \\ z_0 \sim \mathcal{N}(0, 2) \end{cases} \tag{3.68}$$

from which we again simulate a set of 100 observations. Note that, in addition to the non-linearity of μ_z, the density of the law of $y_k|x_k$ is bimodal when $y_k > 0$. Due to these additional difficulties, we therefore expect that using (t, m, s)-nets to estimate the log-likelihood function $\log p(y_{0:T-1})$ is less profitable than for the SV model. This point is confirmed in the Figure 3.2 (right plot) where we show the evolution of the MSE as a function of N. We indeed observe from this plot that the gain of using a number of particles which is a power of two becomes now apparent only for N larger than $10^{3.25} \approx 1\,778$. In addition, it is only for $m \geq 12$ that taking $N = 2^m$ is the fastest way to achieve any further improvement in term of MSE. Finally, the gain of SQMC compared to Monte Carlo techniques can be assessed from Figure 3.2 where we have also represented the Monte Carlo $\mathcal{O}(N^{-1})$ reference line.

To conclude this section it is worth mentioning that to keep the presentation of SQMC simple we have only shown simulations for univariate models. In the multivariate version of SQMC, the resampling step of Algorithm 3.1 (step 12) requires to sort the particles along a Hilbert space filling curve. Since the Hilbert curve is $(1/d)$-Hölder continuous, with d the dimension of the state variable, the estimation problem becomes less smooth as d increases. In light of the observations of this simulation study, this suggests that the gain of restricting N to be powers of the base of the underlying (t, s)-sequence is smaller than for univariate models. This point was confirmed in non reported simulation study conducted for the bivariate version of the SV model (3.67), where the gain of using (t, m, s)-nets as input of SQMC has completely disappeared.

3.6 Conclusion

Together with the works of Yue and Mao (1999) and Hickernell and Yue (2001), the present analysis concludes to show that the results of Owen (1997a,b, 1998) obtained for quadrature rules based on (λ, t, s, m)-nets are in fact true for quadrature rules based on the first N points of scrambled (t, s)-sequences without any restriction on the pattern of N, namely, to sum-up:

1. For any square integrable functions the integration error goes to zero faster than for the classical Monte Carlo estimator;

2. For any square integrable functions the variance of scrambled quadrature rules is bounded by the Monte Carlo variance multiplied by a constant independent of the integrand;

3. The constant in 2. is uniform with respect to the dimension for scrambled $(0, s)$-sequences;

4. For smooth integrands an explicit convergence rate (better than $N^{-1/2}$) can be computed (see Yue and Mao, 1999; Hickernell and Yue, 2001).

In a simulation study, we show that quadratures based on scrambled (λ, t, m, s)-nets outperform those based on nets of arbitrary size when the integrand φ of interest is smooth. More precisely, using scrambled (λ, t, m, s)-nets is for such functions the fastest way to reach any given level of MSE. Nevertheless, as the integrand becomes less smooth, this gain decreases and completely disappears for discontinuous functions.

The second important result proved in this paper is the asymptotic superiority of the sequential quasi-Monte Carlo algorithm proposed by Gerber and Chopin (2014) over standard sequential Monte Carlo methods without any restriction on how the number of particles grows. Since SQMC involves integration of discontinuous functions the behaviour of the MSE when the algorithm takes scrambled (λ, t, m, s)-nets as inputs should not be too different compared to what we would get when scrambled nets of arbitrary size are used. This point is illustrated in a simulation study based in two univariate state-space models and we argue that for multivariate models it is very unlikely to expect any gain of using as input for SQMC only points of scrambled sequences that form (λ, t, m, s)-nets.

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Appendix: Proofs

A Proof of Theorem 3.1

We first prove the following Lemma that plays a key role in the proof of Theorem 3.1.

Lemma 3.1. *Let k and t be two integers such that $k \geq t \geq 0$ and $v_m \in [0, b-1]$, $m = 0, ..., k$. Then,*

$$\sum_{m=t}^{k} v_m b^m \sum_{|u|>0} \sum_{|\kappa|>m-t-|u|} \sigma^2_{u,\kappa} \leq \left(\sum_{m=t}^{k} v_m b^m \right) \sum_{|u|>0} \sum_{|\kappa|>k-t-|u|} \sigma^2_{u,\kappa} + b^k \left(\sum_{|u|>0} \frac{1}{b^{k-t-|u|}} \sum_{|\kappa|\leq k-t-|u|} \sigma^2_{u,\kappa} b^{|\kappa|} \right) \quad (3.69)$$

where we use the convention that empty sums are null.

Proof. For $u \subseteq \mathcal{S}$ and for $l \in \mathbb{Z}$, let $\tilde{\sigma}^2_{u,l} = \sum_{\kappa:|\kappa|=l} \sigma^2_{u,\kappa}$ if $l \geq 0$ and $\tilde{\sigma}^2_{u,l} = 0$ otherwise. To simplify the notations, let $k_t = k - t$ and $v'_m = v_{m+t}$. Then,

$$\sum_{m=t}^{k} v_m b^m \sum_{|u|>0} \sum_{|\kappa|>m-t-|u|} \sigma^2_{u,\kappa} = b^t \sum_{m=0}^{k_t} v'_m b^m \sum_{|u|>0} \sum_{l>m-|u|} \tilde{\sigma}^2_{u,l}.$$

Let $N_t = \sum_{m=t}^{k} v_m b^m$ so that, using (3.56), we have

$$\sum_{m=t}^{k} v_m b^m \sum_{|u|>0} \sum_{|\kappa|>m-t-|u|} \sigma^2_{u,\kappa} = N_t \sigma^2 - b^t \sum_{m=0}^{k_t} v'_m b^m \sum_{|u|>0} \sum_{l\leq m-|u|} \tilde{\sigma}^2_{u,l}. \quad (3.70)$$

In order to study the second term of (3.70), let $u \subseteq \mathcal{S}$ be such that $k_t \geq |u|$. Then,

$$\sum_{m=0}^{k_t} v'_m b^m \sum_{l\leq m-|u|} \tilde{\sigma}^2_{u,l} = \sum_{m=|u|}^{k_t} v'_m b^m \sum_{l=0}^{m-|u|} \tilde{\sigma}^2_{u,l} = \sum_{m=0}^{k_t-|u|} v'_{m+|u|} b^{m+|u|} \sum_{l=0}^{m} \tilde{\sigma}^2_{u,l}.$$

Since

$$\sum_{m=0}^{k_t-|u|} v'_{m+|u|} b^{m+|u|} \sum_{l=0}^{m} \tilde{\sigma}^2_{u,l} = \sum_{l=0}^{k_t-|u|} \tilde{\sigma}^2_{u,l} \sum_{m=l}^{k_t-|u|} v'_{m+|u|} b^{m+|u|},$$

with $b^t \sum_{m=l}^{k_t-|u|} v'_{m+|u|} b^{m+|u|} = N_t - \sum_{m=0}^{l+t+|u|-1} v_m b^m$, we obtain

$$b^t \sum_{m=0}^{k_t} v'_m b^m \sum_{l=0}^{m-|u|} \tilde{\sigma}^2_{u,l} = \sum_{l=0}^{k_t-|u|} \left(N_t - \sum_{m=0}^{l+t+|u|-1} v_m b^m \right) \tilde{\sigma}^2_{u,l}.$$

Therefore, using (3.70) and the convention that empty sums are null,

$$\begin{aligned}
\sum_{m=t}^{k} v_m b^m \sum_{|u|>0} \sum_{|\kappa|>m-t-|u|} \sigma^2_{u,\kappa} &= N_t \sigma^2 - \sum_{|u|>0} \sum_{l=0}^{k_t-|u|} \left(N_t - \sum_{m=0}^{l+t+|u|-1} v_m b^m \right) \tilde{\sigma}^2_{u,l} \\
&= N_t \sum_{|u|>0} \sum_{l>k_t-|u|} \tilde{\sigma}^2_{u,l} + \sum_{|u|>0} \sum_{l=0}^{k_t-|u|} \tilde{\sigma}^2_{u,l} \sum_{m=0}^{l+t+|u|-1} v_m b^m.
\end{aligned}$$

Finally, since $v_m \leq b-1$, we have, for $u \subseteq \mathcal{S}$ such that $k_t \geq |u|$,

$$\begin{aligned}
\sum_{l=0}^{k_t-|u|} \tilde{\sigma}^2_{u,l} \sum_{m=0}^{l+|u|+t-1} v_m b^m &\leq (b-1) \sum_{l=0}^{k_t-|u|} \tilde{\sigma}^2_{u,l} \frac{b^{l+|u|+t}-1}{b-1} \\
&\leq b^k \left(\frac{1}{b^{k-t-|u|}} \sum_{l=0}^{k_t-|u|} \tilde{\sigma}^2_{u,l} b^l \right).
\end{aligned}$$

This shows that

$$\begin{aligned}
\sum_{m=t}^{k} v_m b^m \sum_{|u|>0} \sum_{|\kappa|>m-t-|u|} \sigma^2_{u,\kappa} \leq \left(\sum_{m=t}^{k} v_m b^m \right) \sum_{|u|>0} \sum_{|\kappa|>k-t-|u|} \sigma^2_{u,\kappa} \\
+ b^k \left(\sum_{|u|>0} \frac{1}{b^{k-t-|u|}} \sum_{l \leq k-t-|u|} \tilde{\sigma}^2_{u,l} b^l \right)
\end{aligned}$$

and the proof of the Lemma is complete.

□

To prove the Theorem, and following the proof of Niederreiter (1992, Lemma 4.11, p.56), we decompose $\{\tilde{\mathbf{x}}^n\}_{n=0}^{N-1}$, $N \geq 1$, into scrambled (λ_m, t, m, s)-nets $\tilde{P}_m$, $m = t, ..., (k-t+1)$, and a remaining set $\tilde{P}$ that contains strictly less than b^t points. We recall that k is the largest power of b such that $b^k \leq N$.

To construct this partition of $\{\tilde{\mathbf{x}}^n\}_{n=0}^{N-1}$, let $N = \sum_{m=0}^{k} a_m b^m$ be the expansion of N in base b, with $a_m \in \{0, ..., b-1\}$ and $a_k \neq 0$. Then, let $\tilde{P}_k = \{\tilde{\mathbf{x}}^n\}_{n=0}^{a_k b^k - 1}$ and, for $0 \leq m \leq k-1$, let $\tilde{P}_m$ be the point set made of the $\tilde{\mathbf{x}}^n$'s with $\sum_{h=m+1}^{k} a_h b^h \leq n < \sum_{h=m}^{k} a_h b^h$. By definition of a (t,s)-sequence, $\tilde{P}_m$ is a scrambled (a_m, t, m, s)-nets in base $b \geq 2$ for $m = t, \ldots, k$ while $\tilde{P} = \cup_{m=0}^{t-1} \tilde{P}_m$ has cardinality strictly smaller than b^t.

Using this decomposition of $\{\tilde{\mathbf{x}}^n\}_{n=0}^{N-1}$ we have, using the convention that empty sums are equal to zero,

$$\begin{aligned}
\mathrm{Var}\left(\frac{1}{N}\sum_{n=0}^{N-1}\varphi(\tilde{\mathbf{x}}^n)\right) &= \mathrm{Var}\left(\frac{1}{N}\sum_{\tilde{\mathbf{x}}\in\tilde{P}}\varphi(\tilde{\mathbf{x}}) + \frac{1}{N}\sum_{m=t}^{k}\sum_{\tilde{\mathbf{x}}\in\tilde{P}_m}\varphi(\tilde{\mathbf{x}})\right) \\
&\leq \left\{\frac{1}{N}\mathrm{Var}\left(\sum_{\tilde{\mathbf{x}}\in\tilde{P}}\varphi(\tilde{\mathbf{x}})\right)^{1/2} + \frac{1}{N}\sum_{m=t}^{k}\mathrm{Var}\left(\sum_{\tilde{\mathbf{x}}\in\tilde{P}_m}\varphi(\tilde{\mathbf{x}})\right)^{1/2}\right\}^2 \\
&= \frac{1}{N^2}\mathrm{Var}\left(\sum_{\tilde{\mathbf{x}}\in\tilde{P}}\varphi(\tilde{\mathbf{x}})\right) + \left\{\frac{1}{N}\sum_{m=t}^{k}\mathrm{Var}\left(\sum_{\tilde{\mathbf{x}}\in\tilde{P}_m}\varphi(\tilde{\mathbf{x}})\right)^{1/2}\right\}^2 \\
&\quad + \frac{2}{N}\mathrm{Var}\left(\sum_{\tilde{\mathbf{x}}\in\tilde{P}}\varphi(\tilde{\mathbf{x}})\right)^{1/2}\frac{1}{N}\sum_{m=t}^{k}\mathrm{Var}\left(\sum_{\tilde{\mathbf{x}}\in\tilde{P}_m}\varphi(\tilde{\mathbf{x}})\right)^{1/2}. \quad (3.71)
\end{aligned}$$

For the first term (and in the case where $\tilde{P}$ is not empty) let $\tilde{n} = |\tilde{P}| < b^t$ and note that, using (3.56)-(3.58),

$$\mathrm{Var}\left(\frac{1}{\tilde{n}}\sum_{\tilde{\mathbf{x}}\in\tilde{P}}\varphi(\tilde{\mathbf{x}})\right) = \frac{1}{\tilde{n}}\sum_{|u|>0}\sum_{\kappa}\Gamma_{u,\kappa}\sigma^2_{u,\kappa} \leq \frac{1}{\tilde{n}}b^{t+1}\left(\frac{b+1}{b-1}\right)^{s+1}\sigma^2$$

and therefore,

$$\frac{1}{N^2}\mathrm{Var}\left(\sum_{\tilde{\mathbf{x}}\in\tilde{P}}\varphi(\tilde{\mathbf{x}})\right) \leq \frac{\tilde{n}}{N}\left(b^{t+1}\left(\frac{b+1}{b-1}\right)^{s+1}\right)\frac{\sigma^2}{N} \leq \frac{b^t}{N}\left(b^{t+1}\left(\frac{b+1}{b-1}\right)^{s+1}\right)\frac{\sigma^2}{N}. \quad (3.72)$$

To bound the second term of (3.71) define, for $m \geq t$, $\hat{I}_m = (a_m b^m)^{-1}\sum_{\tilde{\mathbf{x}}\in\tilde{P}_m}\varphi(\tilde{\mathbf{x}})$

if m is such that $a_m \neq 0$ and set $\hat{I}_m = 0$ otherwise. Then,

$$\left\{ \frac{1}{N} \sum_{m=t}^{k} \mathrm{Var} \left(\sum_{\tilde{\mathbf{x}} \in \tilde{P}_m} \varphi(\tilde{\mathbf{x}}) \right)^{1/2} \right\}^2 = \left\{ \frac{1}{N} \sum_{m=t}^{k} \mathrm{Var}(a_m b^m \hat{I}_m)^{1/2} \right\}^2$$

$$= \frac{1}{N^2} \sum_{m=t}^{k} \mathrm{Var}(a_m b^m \hat{I}_m) + \frac{2}{N^2} \sum_{k \geq m > n \geq t} \mathrm{Var}(a_m b^m \hat{I}_m)^{1/2} \mathrm{Var}(a_n b^n \hat{I}_n)^{1/2}. \qquad (3.73)$$

Using (3.59) we have, for $m \geq t$ such that $a_m \neq 0$,

$$\mathrm{Var}(\hat{I}_m) \leq \Gamma_t (a^m b^m)^{-1} \sum_{|u|>0} \sum_{|\kappa| > m-t-|u|} \sigma_{u,\kappa}^2$$

and therefore, using Lemma 3.1,

$$\sum_{m=t}^{k} \mathrm{Var}(a_m b^m \hat{I}_m) \leq \Gamma_t \sum_{m=t}^{k} a_m b^m \sum_{|u|>0} \sum_{|\kappa| > m-t-|u|} \sigma_{u,\kappa}^2 \leq \Gamma_t B_t^{(k)}$$

where $B_t^{(k)}$ is as in the statement of the Theorem. Hence, since $b^k \leq N$,

$$\frac{1}{N} \sum_{m=t}^{k} \mathrm{Var}(a_m b^m \hat{I}_m) \leq \Gamma_t \left(\sum_{|u|>0} \sum_{|\kappa| > k_t - |u|} \sigma_{u,\kappa}^2 + \sum_{|u|>0} \frac{1}{b^{k_t - |u|}} \sum_{|\kappa| \leq k_t - |u|} \sigma_{u,\kappa}^2 b^{|\kappa|} \right).$$

To study the second term of (3.73), let $m > n \geq t$. Then, easy computations show that

$$\frac{a_n a_m b^{n+m}}{\Gamma_t} \mathrm{Var}(\hat{I}_m)^{1/2} \mathrm{Var}(\hat{I}_n)^{1/2} \leq \left(\sum_{|u|>0} \sum_{|\kappa| > m-t-|u|} \sigma_{u,\kappa}^2 \right)^{1/2} \left(\sum_{|u|>0} \sum_{|\kappa| > n-t-|u|} \sigma_{u,\kappa}^2 \right)^{1/2}$$

$$\leq \frac{1}{2} \left(\sum_{|u|>0} \sum_{|\kappa| > m-t-|u|} \sigma_{u,\kappa}^2 + \sum_{|u|>0} \sum_{|\kappa| > n-t-|u|} \sigma_{u,\kappa}^2 \right).$$

Therefore,

$$\frac{2}{\Gamma_t}\sum_{m=t+1}^{k}\sum_{n=t}^{m-1}\mathrm{Var}(a_m b^m \hat{I}_m)^{1/2}\mathrm{Var}(a_n b^n \hat{I}_n)^{1/2}$$

$$\leq \sum_{m=t+1}^{k}\sum_{n=t}^{m-1}\left\{(a_m a_n)^{1/2} b^{\frac{n+m}{2}}\sum_{|u|>0}\sum_{|\kappa|>m-t-|u|}\sigma^2_{u,\kappa} + (a_n a_m)^{1/2} b^{\frac{m+n}{2}}\sum_{|u|>0}\sum_{|\kappa|>n-t-|u|}\sigma^2_{u,\kappa}\right\}$$

$$\leq (b-1)^{1/2}\sum_{m=t+1}^{k}\left(a_m b^{m/2}\sum_{|u|>0}\sum_{|\kappa|>m-t-|u|}\sigma^2_{u,\kappa}\right)\sum_{n=t}^{m-1} b^{\frac{n}{2}}$$

$$+\sum_{m=t+1}^{k} a_m^{1/2} b^{m/2}\left(\sum_{n=t}^{m-1} a_n^{1/2} b^{n/2}\sum_{|u|>0}\sum_{|\kappa|>n-t-|u|}\sigma^2_{u,\kappa}\right)$$

$$\leq c_b\left(\sum_{m=t+1}^{k} a_m b^m \sum_{|u|>0}\sum_{|\kappa|>m-t-|u|}\sigma^2_{u,\kappa}\right)$$

$$+\sum_{m=t+1}^{k} a_m^{1/2} b^{m/2}\left(\sum_{n=t}^{m-1} a_n^{1/2} b^{n/2}\sum_{|u|>0}\sum_{|\kappa|>n-t-|u|}\sigma^2_{u,\kappa}\right) \tag{3.74}$$

with $c_b = \frac{(b-1)^{1/2}}{b^{1/2}-1}$ and where the first term after the last inequality sign is bounded by $B_t^{(k)}$ by Lemma 3.1. For the second term, we have, using Lemma 3.1 (where k is replaced by $m-1$ and b by $b^{1/2}$),

$$\sum_{m=t+1}^{k} a_m^{1/2} b^{m/2}\left(\sum_{n=t}^{m-1} a_n^{1/2} b^{n/2}\sum_{|u|>0}\sum_{|\kappa|>n-t-|u|}\sigma^2_{u,\kappa}\right)$$

$$\leq \sum_{m=t+1}^{k} a_m^{1/2} b^{m/2}\left(\sum_{n=t}^{m-1} a_n^{1/2} b^{n/2}\sum_{|u|>0}\sum_{|\kappa|>m-1-t-|u|}\sigma^2_{u,\kappa}\right.$$

$$\left.+b^{\frac{m-1}{2}}\sum_{|u|>0}\frac{1}{b^{\frac{m-1-t-|u|}{2}}}\sum_{l\leq m-1-t-|u|}\tilde{\sigma}^2_{u,l} b^{l/2}\right)$$

where the right hand side is bounded by

$$c_b\left(\sum_{m=t+1}^{k} a_m b^m \sum_{|u|>0}\sum_{|\kappa|>m-1-t-|u|}\sigma^2_{u,\kappa}\right)$$

$$+ b^{\frac{t}{2}}\sum_{|u|>0} b^{\frac{|u|}{2}}\sum_{m=t+1}^{k} a_m^{1/2} b^{m/2}\sum_{l\leq m-1-t-|u|} b^{\frac{l}{2}}\tilde{\sigma}^2_{u,l}. \tag{3.75}$$

Note that by Lemma 3.1 the term in bracket in the expression (3.75) is bounded by $B_{t+1}^{(k)}$. In addition, in the same spirit as for the derivation of the upper bound in equation (3.69), the second term of (3.75) can be rewritten as

$$b^{\frac{t}{2}} \sum_{|u|>0} b^{\frac{|u|}{2}} \sum_{m=t+1}^{k} a_m^{1/2} b^{m/2} \sum_{l=0}^{m-1-t} b^{\frac{l-|u|}{2}} \tilde{\sigma}^2_{u,l-|u|}$$

$$= b^{t+\frac{1}{2}} \sum_{|u|>0} \sum_{m=0}^{k_t-1} (a'_{m+1} b^m)^{1/2} \sum_{l=0}^{m} b^{\frac{l}{2}} \tilde{\sigma}^2_{u,l-|u|}$$

$$= b^{t+\frac{1}{2}} \sum_{|u|>0} \sum_{l=0}^{k_t-1} b^{\frac{l}{2}} \tilde{\sigma}^2_{u,l-|u|} \sum_{m=l}^{k_t-1} (a'_{m+1} b^m)^{1/2}$$

with $b^{t+\frac{1}{2}} \sum_{m=l}^{k_t} (a'_{m+1} b^m)^{1/2} \leq c_b b^{\frac{k+t}{2}}$. Therefore,

$$b^{\frac{t}{2}} \sum_{|u|>0} b^{\frac{|u|}{2}} \sum_{m=t+1}^{k} a_m b^{m/2} \sum_{l \leq m-1-t-|u|} b^{\frac{l}{2}} \tilde{\sigma}^2_{u,l} \leq c_b b^{\frac{k+t}{2}} \sum_{|u|>0} \sum_{l=0}^{k_t-1} b^{\frac{l}{2}} \tilde{\sigma}^2_{u,l-|u|}$$

$$= c_b b^{\frac{k+t}{2}} \sum_{|u|>0} b^{\frac{|u|}{2}} \sum_{l=0}^{k_t-1-|u|} b^{\frac{l}{2}} \tilde{\sigma}^2_{u,l}$$

$$\leq c_b b^k \sum_{|u|>0} \frac{1}{b^{\frac{k_t-1-|u|}{2}}} \sum_{l=0}^{k_t-1-|u|} b^{\frac{l}{2}} \tilde{\sigma}^2_{u,l}.$$

We conclude the proof using the fact that $(c_1^{1/2} + c_2^{1/2})^2 \leq 2(c_1 + c_2)$.

B Proof of the bound for $t = 0$

To prove the bound for $t = 0$, first note that, in this case, $\tilde{P} = \varnothing$. In addition, a $(0, s)$-sequence in base b exists only if $b \geq s$ (see Dick and Pillichshammer, 2010, Corollary 4.36, p.141) and therefore the gain factors $\Gamma_{u,\kappa}$ are bounded by $\Gamma_0 = e$. Hence, $\sum_{m=0}^{k} \mathrm{Var}\left(a_m b^m \hat{I}_m\right) \leq \Gamma_0 N \sigma^2$ and, from (3.74), the term

$$2 \sum_{m>n\geq t} \frac{\mathrm{Var}(a_m b^m \hat{I}_m)^{1/2} \mathrm{Var}(a_n b^n \hat{I}_n)^{1/2}}{\Gamma_0}$$

is bounded by

$$c_b N \sigma^2 + \sum_{m=1}^{k} a_m^{1/2} b^{m/2} \sum_{n=0}^{m-1} a_n^{1/2} b^{n/2} \sum_{|u|>0} \sum_{|\kappa|>n-|u|} \sigma^2_{u,\kappa} \leq c_b N \sigma^2 + \sigma^2 \sum_{m=t+1}^{k} a_m^{1/2} b^{m/2} \sum_{n=0}^{m-1} a_n^{1/2} b^{n/2}$$

$$\leq 2 c_b N \sigma^2.$$

Using (3.73), we conclude that

$$\mathrm{Var}\left(\frac{1}{N}\sum_{n=0}^{N-1}\varphi(\tilde{\mathbf{x}}^n)\right) \leq \frac{\sigma^2}{N}e\ (1+2c_b) \leq \frac{\sigma^2}{N}e\,(3+2\sqrt{2})$$

because $c_b \leq 1+\sqrt{2}$, $\forall b \geq 2$.

Chapter 4

Bayesian Inference for the Multivariate Extended-Skew Normal Distribution

Joint work with Florian Pelgrin (EDHEC Business School)

Abstract

The (multivariate) extended skew-normal distribution, which belongs to the class of skew-elliptical distributions, allows for accommodating with additional parameters raw data which are skewed and heavy tailed while being tractable and parsimonious, and having at least three appealing statistical properties, namely closure under conditioning, affine transformations, and marginalization. In this paper we propose a Bayesian estimation approach based on a tempered sequential Monte Carlo (SMC) algorithm. The practical implementation of each step of the algorithm is discussed and the elicitation of the prior distributions takes into consideration some unusual behaviour of the likelihood function and the corresponding Fisher information matrix. Using Monte Carlo simulations, we provide strong evidence regarding the statistical performances of the SMC sampler as well as some new insights regarding the parametrizations (latent representation and convolution representation) of the extended skew-normal distributions. A generalization to the extended skew-normal sample selection model is also presented. Finally we proceed with the analysis of two real datasets.

Keywords: Bayesian estimation; Bayes factor; Sequential Monte Carlo; Skew-elliptical distributions

4.1 Introduction

Recent years have seen a growing interest for flexible parametric families of non-normal distributions that can accommodate with additional parameters the skewness and the kurtosis. This is especially important e.g. in health, finance, environmental data which are often skewed and heavy tailed. For instance, these two features of health (-care) expenditures have fundamental implications in topics related to risk adjustments, program and treatment evaluations, or insurance choices. In this respect, the application of the skew-elliptical family of distributions (i.e., all non-symmetric distributions obtained from an elliptical distribution) has been put forward in the literature and for good reasons. On the one hand, this family (or certain distributions of this family) has, at least, three appealing properties: closure under conditioning, affine transformations, and marginalization.[1] On the other hand, these parametric distributions appear in the natural and important context of selection models (Heckman, 1976; Copas and Li, 1997; Arnold and Beaver, 2002). This last feature is particularly relevant in various research topics.[2]

Within the class of skew-elliptical distributions, the (multivariate) extended skew-normal distribution appears in different areas of statistical theory, e.g. Bayesian statistics (O'Hagan and Leonard, 1976), regression analysis (Copas and Li, 1997) or graphical models (Capitanio and Stanghellini, 2003). The extended skew-normal family of distributions finds its origins in the seminal paper of Azzalini (1985) and has then been developed and studied by Arnold et al. (1993), Arnold and Beaver (2000), Capitanio and Stanghellini (2003). Such a family of distributions has at least two equivalent representations. On the one hand, it can be defined by hidden truncation (and/or selective reporting) using normal component densities, say $\mathbf{Y} \stackrel{d}{=} (\boldsymbol{\xi} + \widetilde{\mathbf{Y}}_1 | \lambda + \boldsymbol{\alpha}' \widetilde{\mathbf{Y}}_1 > Z_1)$ where λ, $\boldsymbol{\alpha}$ and $\boldsymbol{\xi}$ denote respectively the shift, shape and location parameter, and $\widetilde{\mathbf{Y}}_1 \in \mathbb{R}^d$ and $Z_1 \in \mathbb{R}$ are independent normally distributed random variables. On the other hand, an equivalent representation is given by the convolution between a multivariate normal distribution, $\widetilde{\mathbf{Y}}_3$, and a truncated standard normal random variable, Z_3, say $\mathbf{Y} \stackrel{d}{=} \widetilde{\mathbf{Y}}_3 + \boldsymbol{d} Z_3$. The derivation and statistical properties of extended skew-normal distributions make it a natural candidate to model skewed and (leptokurtic, platikurtic) mesokurtic data generating

[1] Moreover, Fang (2003, 2005b,a) argues that usual test statistics can be used with either the same distributions or similar ones (as if they were based on the normal assumption).

[2] The usual (parametric) statistical modelling assumes that a random sample is drawn from a (symmetric) probability density function (that depend on a vector of unknown parameters) and that realizations can be observed in order to make inference about this parameter vector. However there are many situations in which a random sample might not be available. For instance, this occurs in two important situations in health economics or medical statistics: (i) when the observed data are obtained from a selected portion of the population of interest (e.g., individuals who benefits from a specific treatment); (ii) when the observed data are drawn from a given distribution but have been truncated with respect to some hidden co-variables.

processes. However, as pointed out by Arellano-Valle et al. (2006), statistical inference of (multivariate) skew-elliptical distributions and thus of the multivariate extended skew-normal family of distributions is still mostly unsolved (even in the univariate case).

In this paper we propose a new algorithm for the multivariate extended skew-normal distribution. Bayesian analysis of some families of skew-elliptical distributions has been proposed in the literature. However, to the best of our knowledge, such Bayesian analysis mainly focuses on the (multivariate) skew-normal or skew-t distribution, and some mixtures of these distributions using objective priors-based methods, Gibbs sampling or population Monte Carlo. Indeed, Liseo and Loperfido (2006) propose a Bayesian estimation of the univariate skew-normal distribution based on objective priors whereas Wiper et al. (2008) analyze the half-normal and half-t cases, and Branco et al. (2013) focus on the skew-t distribution.[3] On the other hand, Cabral et al. (2012) propose a full Bayesian estimation of a mixture of skew-normal densities while Früwirth-Schnatter and Pyne (2010) provide a Gibbs sampler to estimate a mixture of skew-normal and skew-t densities. As an alternative to the Gibbs sampler, Liseo and Parisi (2013) advocate the application of a Population Monte Carlo (PMC) algorithm for missing data (Celeux et al., 2004) in order to sample from the posterior distribution of the skew-normal model.[4]

In contrast, our methodology rests on (tempered) sequential Monte Carlo (Del Moral et al., 2006). Briefly speaking, the general class of sequential Monte Carlo algorithms iterates importance sampling steps, resampling steps and Markov kernel transitions in order to recursively approximate a sequence of distributions by making use of a sequence of weighted particle systems. In this respect, our methodology is clearly motivated by three arguments. First, the standard maximum likelihood estimation method presents some severe anomalies that can be (partially) overcome by a full Bayesian approach. Second, the application of a Gibbs sampler turns out to be infeasible for the extended skew-normal distribution. To further understand this point, consider the convolution-based approach of the extended skew-normal distribution (P2). A natural idea to sample from the posterior distribution is to implement a Gibbs sampler in which the hidden random variable Z_3 is an extra parameter. Nevertheless the support of the hidden variable depends on one parameter of interest and, consequently, the posterior distribution in the augmented space does not satisfy the positivity condition (see Robert and Casella, 2004, chapter 9).[5]

[3]Fung and Senata (2010), and Ferraz and Mourra (2012) consider the bivariate skew-normal distribution.

[4]Note that the algorithm of Liseo and Parisi (2013) can be applied in the case of the multivariate skew-normal family of distributions. However our adaptive (tempered) Sequential Monte Carlo approach nests their population Monte Carlo algorithm and presents some others advantages (see further).

[5]Some other features of the Gibbs sampler for the skew-normal distribution are discussed in Liseo and Parisi (2013).

Third, sequential Monte Carlo (SMC) methods are a general class of algorithms, which contains population Monte Carlo samplers. The greater generality of SMC allows to build more efficient algorithms and ought to be preferred with Markov chain Monte Carlo (MCMC) methods in order to sample from complicated distributions. Compared to MCMC, it is easier to make SMC algorithms adaptive in the sense that they can be adjusted sequentially (using past simulations in order to improve their performance in subsequent iterations) and automatically to the problem at hand. In so doing, SMC samplers are efficient to sample from high dimensional distributions.[6]

Our paper makes the following contributions. First, as explained above, we provide an adaptive tempered sequential Monte Carlo algorithm for the multivariate extended skew-normal family of distributions. Second, we provide a formal proof for the lack of identification of the maximum likelihood estimator in the case of the univariate extended skew-normal distribution. Third, we conduct a (comprehensive) Monte Carlo study using different data generating processes (univariate extended skew-normal distributions and extended skew-normal regressions models with missing data). Among others, this provides some new insights regarding the implications of both hidden truncation-based and convolution-based parametrization. Finally, we present a new class of sample selection models, namely the extended skew-normal sample selection (or Tobit-type) models.

The rest of the paper is organized as follows. Section 4.2 defines two equivalent representations of multivariate skew-normal random vectors, review some useful properties of this class of distributions, and discuss some unpleasant features of the maximum likelihood function. Section 4.3 describes our tempered sequential Monte Carlo algorithms. Section 4.4 presents some Monte Carlo simulations regarding the inference of univariate and bivariate extended skew-normal distributions as well as some regressions with missing data. Moreover we discuss the testing and model selection problems. Section 4.5 deals with an application using a financial data set (Liseo and Parisi, 2013). The last section provides some concluding remarks.

4.2 The extended skew-normal distribution

In this section we first define the extended skew-normal (ESN) distribution using two different parametrizations. Then we review some appealing properties of this class of distributions, especially in the light of the subsequent derivations of this paper. Finally we provide a new theoretical justification for the unsatisfactory behaviour of the maximum likelihood estimator of the ESN distribution.

[6]Note that the identification issues discussed above imply that some parameters may be highly correlated, which is always challenging for MCMC methods.

4.2.1 Definition and main properties

We consider (among others) two parametrizations of the ESN distribution. The first parametrization, denoted P1, is based on hidden truncation (and/or selective reporting) using normal component densities whereas the second parametrization, denoted P2, rests on the convolution of a multivariate normal distribution with a truncated standard normal variable (which is distributed independently).

Definition 4.1. *A random vector* $\mathbf{Y}$ *is said to have a d-dimensional extended skew-normal distribution, denoted* $\mathbf{Y} \sim \mathcal{ESN}_d(\boldsymbol{\xi}, \Sigma, \boldsymbol{\alpha}, \lambda)$ *(P1), with covariance (correlation) matrix* Σ*, shape parameter* $\boldsymbol{\alpha}$*, and shift parameter* λ*, if*

$$\mathbf{Y} \overset{d}{=} \left(\boldsymbol{\xi} + \widetilde{\mathbf{Y}}_1 | \lambda + \boldsymbol{\alpha}'\widetilde{\mathbf{Y}}_1 > Z_1\right), \qquad \begin{pmatrix}\widetilde{\mathbf{Y}}_1 \\ Z_1\end{pmatrix} \sim \mathcal{N}_{d+1}\left(\begin{pmatrix}\mathbf{0} \\ 0\end{pmatrix}, \begin{pmatrix}\Sigma & \mathbf{0} \\ \mathbf{0} & 1\end{pmatrix}\right) \tag{4.76}$$

where $\mathcal{N}_{d+1}(\boldsymbol{\mu}, B)$ *denotes the* $(d+1)$*-dimensional Gaussian distribution with mean* $\boldsymbol{\mu}$ *and variance-covariance matrix* B*. Its density function is defined to be:*

$$f_Y(\mathbf{y}) = \phi_d\left(\mathbf{y}, \boldsymbol{\xi}, \Sigma\right) \frac{\Phi(\lambda + \boldsymbol{\alpha}'(\mathbf{y} - \boldsymbol{\xi}))}{\Phi\left(\lambda / c_0\right)}, \quad c_0 = \sqrt{1 + \boldsymbol{\alpha}'\Sigma\boldsymbol{\alpha}} \tag{4.77}$$

where $\phi_d\left(\cdot, \boldsymbol{\mu}, B\right)$ *is the density of the d-dimensional normal distribution with mean* $\boldsymbol{\mu}$ *and covariance (correlation) matrix* B *and* $\Phi(\cdot)$ *is the cumulative density function (cdf) of the* $\mathcal{N}_1(0,1)$ *distribution.*

On the other hand, the ESN distribution can be defined from a convolution.

Definition 4.2. *A random vector* $\boldsymbol{Y}$ *is said to have a d-dimensional extended skew-normal distribution, denoted* $\mathbf{Y} \sim \mathcal{ESN}_d(\boldsymbol{\xi}, \Omega, \boldsymbol{d}, c)$ *(P2), if*

$$\mathbf{Y} \overset{d}{=} \widetilde{\mathbf{Y}}_3 + \boldsymbol{d}Z_3$$

where $-Z_3 \sim \mathcal{TN}_c(0,1)$*, the* $\mathcal{N}_1(0,1)$ *distribution truncated to* $(-\infty, c]$*, and* $\widetilde{\mathbf{Y}}_3 \sim \mathcal{N}_d(\mathbf{0}, \Omega)$*. Its probability density function is defined to be:*

$$f_Y(\mathbf{y}) = \phi_d\left(\mathbf{y}, \boldsymbol{\xi}, \Omega + \mathbf{d}\mathbf{d}'\right) \frac{\Phi\left(c_0\left\{c + \mathbf{d}'\left[\Omega + \mathbf{d}\mathbf{d}'\right]^{-1}\left(\mathbf{y} - \boldsymbol{\xi}\right)\right\}\right)}{\Phi\left(c\right)}.$$

Several points are worth commenting. First, the ESN distribution belongs to the families of (multivariate unified) skew-elliptical distributions proposed by Arnold and Beaver (2002), Domínguez-Molina et al. (2003), Fang (2003), and Arellano-Valle and Genton (2010).[7] Alternatively, using P2, the ESN distribution can be viewed as the result of the family of distributions proposed by Sahu et al. (2003).

[7]The family of skew-ellliptical distributions based on hidden truncation (Arnold and Beaver, 2002; Arellano-Valle et al., 2006) can be defined as follows. Let $\mathbf{X} = (\mathbf{Y}, \mathbf{Y}_0)$ be an elliptic vector

Irrespective of the parametrization, the ESN distribution generalizes the multivariate skew-normal distribution (Azzalini and Dalla Valle, 1996) and thus the Gaussian distribution. More specifically, when the shift parameter λ is set to zero, one obtains the (multivariate) SN distribution. On the other hand, the standard normal distribution results from the nullity of the shape or directional parameter vector $\boldsymbol{\alpha}$. As explained in Section 4.2.2, this constraint on the shape parameter vector has some strong implications on inference. Indeed, the Fisher information matrix of the ESN (SN) distribution is singular: this prevents a straightforward application of standard likelihood-based methods to test the null hypothesis of normality. The problem is even made worse by the parameter λ, which indexes the distribution in the case of nonnormality (nuisance parameter).

Second, the choice of the parametrization might be critical for both estimation and simulations of ESN random vectors.[8] As to be expected, in a Bayesian perspective, different parametrizations lead to alternative choices of prior distributions and thus model distributions (see Section 4.3). In addition, it has also some key insights on Monte Carlo algorithms in order to generate ESN random vectors. Indeed, while the stochastic representation (4.76) might be in favour of an acceptance-rejection algorithm, this is quite an inefficient sampling method since the probability to accept a value $\tilde{\mathbf{y}}_1$ of $\tilde{\mathbf{Y}}_1$ is $\Phi(\lambda/c_0)$, which may be too small for negative values of λ. In contrast, taking the convolution-based parametrization P2, sampling an ESN random vector requires generating a multivariate Gaussian vector and an univariate truncated Gaussian random variable—this can be efficiently conducted, e.g. by implementing the algorithm proposed by Chopin (2011).

Third, one key feature of the ESN distribution over the SN distribution is that the

in $\mathbb{R}^{k+p}$, where k is the dimension $\mathbf{Y}$. The density of $\mathbf{X}$ is given by (Fang and Zhang, 1990):

$$\psi_{(k+p)}(\mathbf{x}, \boldsymbol{\mu}, \Omega) = |\Omega|^{-\frac{1}{2}} g^{(k+p)}\left[(\mathbf{x}-\boldsymbol{\mu})'\Omega^{-1}(\mathbf{x}-\boldsymbol{\mu})\right]$$

where

$$g^{(m)}(x) = \frac{\Gamma\left(\frac{m}{2}\right)}{\pi^{\frac{m}{2}}} \frac{g(x,m)}{\int_0^{+\infty} r^{\frac{m}{2}-1} g(r,m) dr}$$

is the density generator and $g(x,m)$ is a nonincreasing function from $\mathbb{R}^+$ in $\mathbb{R}^+$ such that the integral in the previous expression is finite. We can define (Arellano-Valle et al., 2006) a SED as the law of $\mathbf{Z}$ where

$$\mathbf{Z} \stackrel{d}{=} (\mathbf{Y} | h(\mathbf{Y}, \mathbf{Y}_0) \in C)$$

with $h : \mathbb{R}^{k+p} \to \mathbb{R}^p$ and $C \subset \mathbb{R}^p$. Provided that the distribution of $\mathbf{Z}$ admits a density, one obtains:

$$f_{\mathbf{Z}}(\mathbf{z}) = \psi_k(\mathbf{z}, \boldsymbol{\xi}, \Sigma) \frac{\Pr(h(\mathbf{Y}, \mathbf{Y}_0) \in C | \mathbf{Y} = \mathbf{z})}{\Pr(h(\mathbf{Y}, \mathbf{Y}_0) \in C)}$$

where $\psi_k(\cdot, \boldsymbol{\xi}, \Sigma)$ is the density of the marginal distribution of $\mathbf{Y}$. For singular elliptical-contoured distributions, see Díaz et al. (2002)

[8] A discussion about identifiability of some parametrizations is given by Castro et al. (2010) for the extended skew-normal distribution.

former has an extra parameter that allows for a larger range of values for skewness and kurtosis.[9] For instance, using the moment generating function of Domínguez-Molina et al. (2003), we conduct a numerical analysis for the univariate ESN which provides evidence that the skewness coefficient is bounded by 2 (in absolute value) while the kurtosis coefficient varies roughly between 2.75 and 7. In contrast, Azzalini (1985) points out that the skewness is smaller (in absolute value) than 0.995 and that the kurtosis lies between 3 and 3.87.[10]

Fourth, the ESN distribution has three familiar and useful properties, especially for regression-type models. It is closed under affine transformations, conditioning and marginalization. On the one hand, ESN random vectors share the affine transformation of normal random vectors. In particular, let A denote an $d \times d$ non-singular matrix and $\tilde{\boldsymbol{\xi}} \in \mathbb{R}^d$. Then, taking (4.76), one obtains $\tilde{\boldsymbol{\xi}} + A'\mathbf{Y} \sim \mathcal{ESN}_d(\tilde{\boldsymbol{\xi}} + A'\boldsymbol{\xi}, A'\Sigma A, A^{-1}\boldsymbol{\alpha}, \lambda)$. On the other hand, if an ESN vector is partitioned into two components, the conditional distribution of one component given the other is extended skew normal and each component is marginally extended skew-normal distributed.[11] For sake of completeness, Proposition 4.1 due to Fang (2003) and Domínguez-Molina et al. (2003) reports the closure of the ESN distribution under conditioning and marginalization.

Proposition 4.1. *Assume that* $\mathbf{Y} \sim \mathcal{ESN}_d(\boldsymbol{\xi}, \Sigma, \boldsymbol{\alpha}, \lambda)$. *Partition* $\mathbf{Y}$, $\boldsymbol{\xi}$, $\boldsymbol{\alpha}$ *and* Σ *as* $\mathbf{Y} = (\mathbf{Y}_1, \mathbf{Y}_2)'$, $\boldsymbol{\epsilon} = (\boldsymbol{\epsilon}_1, \boldsymbol{\epsilon}_2)'$, $\boldsymbol{\alpha} = (\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2)'$ *and* $\Sigma = \left(\begin{smallmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{smallmatrix}\right)$ *where* $\mathbf{Y}_i$, $\boldsymbol{\xi}_i$ *and* $\boldsymbol{\alpha}_i$ *are* $m_i \times 1$ *and* Σ_{ii} *is* $m_i \times m_i$. *Then,*

$$\mathbf{Y}_i \sim \mathcal{ESN}_{m_i}(\boldsymbol{\xi}_i, \Sigma_{ii}, c_i\tilde{\boldsymbol{\alpha}}_i, c_i\lambda), \qquad (\mathbf{Y}_i|\mathbf{Y}_j = \mathbf{y}_j) \sim \mathcal{ESN}_{m_i}(\boldsymbol{\xi}_i^c, \Sigma_{ii.1}, \boldsymbol{\alpha}_i, \lambda_i)$$

where $c_i = (1 + \boldsymbol{\alpha}_j'\Sigma_{i.1}\boldsymbol{\alpha}_j)^{-1/2}$, $\boldsymbol{\xi}_i^c = \boldsymbol{\xi}_i + \Sigma_{ij}\Sigma_{jj}^{-1}(\mathbf{y}_j - \boldsymbol{\xi}_j)$, $\Sigma_{ii.1} = \Sigma_{ii} - \Sigma_{ij}\Sigma_{jj}^{-1}\Sigma_{ji}$, $\tilde{\boldsymbol{\alpha}}_i = \boldsymbol{\alpha}_i + \Sigma_{ii}^{-1}\Sigma_{ij}\boldsymbol{\alpha}_j$ *and* $\lambda_i = \lambda + \tilde{\boldsymbol{\alpha}}_j(\mathbf{y}_j - \boldsymbol{\xi}_j)$.

See Fang (2003) or Domínguez-Molina et al. (2003) for a proof.

Finally, the stochastic representation (4.76) of ESN random vectors leads to the following expression of the cumulative density function (henceforth, cdf):

$$\mathbb{P}(\mathbf{Y} \leq \mathbf{y}) = \frac{\Phi_{d+1}(\mathbf{y} - \boldsymbol{\xi}, \Sigma, \boldsymbol{\alpha}, \lambda)}{\Phi(\lambda/c_0)}$$

[9] It is worth noting that replacing $\boldsymbol{\alpha}$ by $\boldsymbol{\alpha}' = -\boldsymbol{\alpha}$ does neither modify the value of the kurtosis nor the absolute value of the skewness coefficient since, from the density (4.77). Indeed, if $\mathbf{Y}' \sim \mathcal{ESN}_d(\boldsymbol{\xi}, \Sigma, -\boldsymbol{\alpha}, \lambda)$, then, $\forall \mathbf{y} \in \mathbb{R}^d$, $f_{\mathbf{Y}'}(\mathbf{y}) = f_{\mathbf{Y}}(-\mathbf{y})$ where $\mathbf{Y} \sim \mathcal{ESN}_d(\boldsymbol{\xi}, \Sigma, \boldsymbol{\alpha}, \lambda)$.

[10] In a multivariate setting, one can use the multivariate skewness and kurtosis measures for singular distributions proposed by Mardia (1970) and Ardanuy and Sanchez (1993). Using Mardia (1970)'s results, upper and lower bounds of these measures can be derived. In the case of the multivariate extended skew-t distributions, see Arellano-Valle and Genton (010b).

[11] Taking Proposition 4.1, it is worth commenting that an ESN random vector might have some components which are jointly Gaussian since e.g. $\mathbf{Y}_i \sim \mathcal{N}_{m_i}(\boldsymbol{\xi}_i, \Sigma_{ii})$ if $\boldsymbol{\alpha}_i + \Sigma_{ii}^{-1}\Sigma_{ij}\boldsymbol{\alpha}_j = \mathbf{0}_{m_i}$.

with $\Phi_{d+1}(\mathbf{a}, \Sigma, \boldsymbol{\alpha}, \lambda) = \mathbb{P}\left(\widetilde{\mathbf{Y}}_2 \leq \mathbf{a}, Z_2 \leq \lambda\right)$ where

$$(\widetilde{\mathbf{Y}}_2, Z_2) \sim \mathcal{N}_{d+1}\left(\begin{pmatrix}\mathbf{0}\\ 0\end{pmatrix}, \begin{pmatrix}\Sigma & -\Sigma\boldsymbol{\alpha}'\\ -\boldsymbol{\alpha}'\Sigma & c_0^2\end{pmatrix}\right).$$

Notably the evaluation of the cdf of the d-dimensional ESN distribution has the same complexity as the computation of the cdf of the $(d+1)$-dimensional Gaussian distribution, for which efficient methods are available (e.g., see Huguenin et al., 2008). It turns to be very useful in practice since, for instance, the cdf of the ESN distribution arises naturally when deriving the expression of the likelihood function in the presence of missing data (see further).

4.2.2 Log-likelihood function

Since our methodology rests on Bayesian estimation and thus on the posterior distribution associated to the ESN-based model, it is fundamental to study the statistical properties of the (log-) likelihood function. This might provide some useful insights in order to determine the prior distributions and thus challenge some identified anomalies regarding the (log-) likelihood function (i.e., to correct at least partially the odd behavior of the likelihood function with external information). In this respect we discuss some key issues regarding the (log-) likelihood function and the maximum likelihood estimator of ESN distributions. For sake of exposition, we concentrate on the univariate extended skew-normal distribution.

Maximum likelihood estimation of ESN distributions is challenging and quite difficult to manage. More specifically, it is widely acknowledged that (i) there are no closed form expressions for the maximum likelihood estimator (MLE), (ii) the MLE of α can be infinite even in very simple settings, (iii) the multimodality of the log-likelihood profile (and thus local solutions) can not be ruled out and (iv) there exists an inflexion point at $\alpha = 0$.[12] In particular, the Fisher information matrix tends to be singular as α goes toward zero irrespective of the λ parameter. Note that, in this case, the ESN distributions are no longer indexed by the normal cumulative density functions and, consequently, the rank of the information matrix might be at least two less than its full rank. On the other hand, the presence of a stationary point (e.g., using the profile log-likelihood for the α parameter) and of multiple modes generally cause numerical issues.

While these issues have been outlined in the literature, to the best of our knowledge, there is not yet a formal proof of the near unidentifiability of the log-likelihood function and the λ parameter. Therefore we show in Proposition 4.2 that the presence of the shift parameter λ in P1 might lead to local maxima for the maximum likelihood estimator of the univariate extended skew-normal distribution.[13] The

[12] The first two points are also shared by the SN distribution. See Azzalini and Capitanio (1999).
[13] The same proposition holds for P2.

starting point goes as follows. Irrespective of the data and for all $l \in \mathbb{R}$, the ESN distribution admits a stationary point at $\theta^l_{n,G} := (\boldsymbol{\xi}_{n,G}, \Sigma_{n,G}, \mathbf{0}_d, l)$, where $\boldsymbol{\xi}_{n,G}$ and $\Sigma_{n,G}$ are the maximum likelihood estimator of $\boldsymbol{\xi}$ and Σ under the Gaussian assumption. In so doing, if this stationary point is an inflexion point when we impose the λ parameter to be zero (Azzalini and Capitanio, 1998), the problem becomes even more severe when λ is a free parameter as stated in Proposition 4.2.

Proposition 4.2. *Let $Y_1, ..., Y_n$ be n i.i.d. random variables, $Y_1 \sim \mathcal{ESN}_1(\xi, \sigma^2, \alpha, \lambda)$ with $\alpha \neq 0$. Let $\theta^l_{n,G} = (\xi_{n,G}, \sigma^2_{n,G}, 0, l)$ with $\xi_{n,G} = \frac{1}{n}\sum_{i=1}^n Y_i$ and $\sigma^2_{n,G} = \frac{1}{n}\sum_{i=1}^n Y_i^2 - \xi^2_{n,G}$. Let $L_n(\theta)$ denote the log-likelihood function. Then,*

1. *With probability one, there exists $l^* \in \mathbb{R}$ such that $L_n(\theta^l_{n,G})$ is a local maximum of L_n for all $l \leq l^*$;*

2. *With strictly positive probability, $L_n(\theta^l_{n,G}) = L_n(\theta_n)$, $l \in \mathbb{R}$, where $\theta_n \neq \theta^l_{n,G}$ is a global maximizer of L_n.*

See Appendix A for a proof.

The first result of Proposition 4.2 has an intuitive interpretation. When $\alpha = 0$, the value of the log-likelihood function is insensitive to any change of the λ parameter and thus any small deviation of α leads to large deviations from the true log-likelihood value (since the estimate λ was initially far from its true unknown value). As a direct consequence, a small deviation from $\theta^l_{n,G}$ in any direction reduces the value of the likelihood. The second part of Proposition 4.2 is more puzzling because it implies that, with a positive (but decreasing with n) probability, the likelihood function does not allow to discriminate between the Gaussian and the ESN model. This is a particularly severe anomaly of the likelihood function because it implies that the MLE may be not uniquely defined.

4.3 Bayesian analysis of the ESN distribution

In this section we show how to estimate the parameters of the two parametrizations of ESN distributions using Sequential Monte Carlo (Del Moral et al., 2006). This general class of algorithms iterates importance sampling steps, resampling steps and Markov kernel transitions in order to recursively approximate a sequence of distributions by making use of a sequence of weighted particles which represents the current distribution. Notably we make use of a tempered version of a sequential Monte Carlo sampler (Del Moral et al., 2006). For sake of presentation, we first provide an overview of our methodology. Then we present the choice of prior distributions. Finally the complete algorithm is exposed and each step is commented separately through comprehensive instructions that correspond exactly to our implementation.

4.3.1 An overview

Let θ be the vector whose components are the parameter of the model (either under P1 or under P2), $f(\mathbf{z}_{1:n}|\theta)$ be the likelihood function where $\mathbf{z}_{1:n} = (\mathbf{z}_1, ..., \mathbf{z}_n)$ is the set of observations and $\pi(\theta)$ be the prior distribution of the parameters which is either $\pi_{\mathrm{P1}}(\theta)$ under P1 or $\pi_{\mathrm{P2}}(\theta)$ under P2. Using these notations, the posterior distribution we want to sample from is given by

$$\pi(\theta|\mathbf{z}_{1:n}) \propto f(\mathbf{z}_{1:n}|\theta)\pi(\theta).$$

As pointed out by Del Moral et al. (2006), sequential Monte Carlo samplers are relevant when there is no fully-eligible proposal distribution, say $\eta_1(\theta)$, in order to implement the importance sampler. The SMC sampler requires to define a sequence of distribution $\{\pi_t(\theta)\}_{t=1}^T$ such that (i) $\pi_T(\theta) = \pi(\theta|\mathbf{z}_{1:n})$, the posterior distribution, and (ii) $\pi_1(\theta)$ is easy to approximate with a proposal distribution $\eta_1(\theta)$ using importance sampling.

The basic idea of a SMC algorithm is first to compute the Monte Carlo approximation $\pi_1^N(\mathrm{d}\theta) = \sum_{m=1}^N W_1^m \delta_{\theta_1^m}(\mathrm{d}\theta)$ of $\pi_1(\theta)\mathrm{d}\theta$ and then, using resampling and propagation steps, to move from $\pi_1^N(\mathrm{d}\theta)$ to $\pi_2^N(\mathrm{d}\theta) = \sum_{m=1}^N W_2^m \delta_{\theta_2^m}(\mathrm{d}\theta)$, a Monte Carlo approximation of $\pi_2(\theta)\mathrm{d}\theta$. Informally, if π_1^N is a good approximation of π_1 and if π_2 is close to π_1, then one may expect π_2^N to be close to π_2, and so on.

To shed more light on the importance sampling, resampling and propagation steps, suppose that one has, at iteration t, a weighted sample $\{(W_t^m, \theta_t^m)\}_{m=1}^N$ which approximates $\pi_t(\mathrm{d}\theta)$, then $\left\{(W_{t+1}^m, \theta_t^m)\right\}_{m=1}^N$ approximates $\pi_{t+1}(\mathrm{d}\theta)$ with

$$W_{t+1}^m = \frac{w_{t+1}^m}{\sum_{j=1}^N w_{t+1}^j}, \qquad w_{t+1}^m = W_t^m \frac{\pi_{t+1}(\theta_t^m)}{\pi_t(\theta_t^m)}. \tag{4.78}$$

This is the *importance sampling step*. Notably, if particles are only generated at date $t = 1$ and then reweighed using (4.78), the algorithm is an importance sampling algorithm with $\eta_1(\theta)$ as the importance distribution. In contrast, if η_1 is a poor approximation of π, then only a few particles are in the support of the target distribution that receives a high density. Such a weight degeneracy is then controlled by interspersing resample (*resampling step*) and thus keeping track of the particle approximation. Finally, to diversify the resampled system, which may contain multiple copies of many particles, and thus "visit" as much as possible the support of the target distribution, new particles are generated using a Markov kernel which is constructed through a parametric family that depends on the parameters of interest. This is the *moving* or *propagation step*. In addition to the initial smooth sequence of distributions, these three steps are further detailed and amended in the tempered SMC algorithm proposed below.

4.3.2 A default Prior specification

Before presenting the proposed tempered SMC algorithm, we discuss the choice of our prior distributions for both parametrizations of the multivariate ESN distribution. In contrast to the standard approach of default prior distributions, and in the spirit of Gelman et al. (2008), we propose some prior specifications that embed enough information to circumvent the anomalies of the log-likelihood function listed in Section 4.2.2.

On the one hand, the $(\boldsymbol{\xi}, \Sigma, \boldsymbol{\alpha}, \boldsymbol{\lambda})$-parametrization (P1) of ESN random vectors must tackle two issues, namely the potential existence of multiple modes and the identification (estimation) of the truncation point, that are related to the identification of the λ parameter. First the multi-modality of the log-likelihood function might be attenuated by setting a prior that put less weight on very negative values of λ. Second, as argued in Section 4.2.2, values of λ such that the truncation point exceeds a certain threshold, say $\frac{|\lambda|}{c_0} > 2$, are difficult to identify and therefore, both to avoid extreme estimates of λ and to facilitate its identification in this region of the parameter space, it is important to chose a prior $\pi(\mathrm{d}\lambda|\Sigma, \boldsymbol{\alpha})$ that put small weights on $\{l \in \mathbb{R} : |l|/c_0 > 2\}$. In so doing we propose to consider a conditional normal prior distribution with mean zero and variance c_0^2, $\lambda|(\Sigma, \boldsymbol{\alpha}) \sim \mathcal{N}_1(0, c_0^2)$. This naturally leads to choose a normal-inverse Wishart distribution as a prior for $(\boldsymbol{\xi}, \Sigma)$, which is the conjugate prior for Gaussian models (e.g., see Gelman et al., 2004). Note that it turns to ease to some extent the Bayesian model selection procedure (see Section 4.3.4). Hence

$$\pi(\boldsymbol{\xi}, \Sigma|\boldsymbol{\alpha}) \propto \exp\left(-\frac{1}{2}\mathrm{tr}(V\Sigma^{-1}) - \frac{\kappa}{2}(\boldsymbol{\xi} - \boldsymbol{\xi}_0)'\Sigma^{-1}(\boldsymbol{\xi} - \boldsymbol{\xi}_0)\right)|\Sigma|^{-\frac{\nu+d+2}{2}} \tag{4.79}$$

where V is a $d \times d$ positive definite matrix, κ and ν are real such that $\nu > d+3$. This last condition ensures that the prior for Σ has a mean and that all its components has finite variance. Finally, one can choose a vague prior for $\boldsymbol{\alpha}$, e.g. $\boldsymbol{\alpha} \sim \mathcal{N}_d(\boldsymbol{\mu}_{\boldsymbol{\alpha}}, \sigma^2_{\boldsymbol{\alpha}} I_d)$ with $\sigma^2_{\boldsymbol{\alpha}}$ large and I_d the $d \times d$ identity matrix. Note that in practice it is likely to have information on the sign of α_i, $i = 1, ..., d$, through information about the asymmetry of the full conditional distribution of Y_i. This prior knowledge can be incorporated in the Bayesian analysis by taking $\boldsymbol{\mu}_{\boldsymbol{\alpha}} \neq \mathbf{0}_d$.

On the other hand, the $(\boldsymbol{\xi}, \Omega, \boldsymbol{d}, c)$-parametrization shares the same issues as the P1-parametrization since $c = \frac{\lambda}{c_0}$. In addition, since $\mathbf{Y}$ is defined by $\mathbf{Y} \overset{d}{=} \boldsymbol{\xi} + \mathbf{d}Z_3 + \Omega^{1/2}\widetilde{\mathbf{Y}}_3$ where $-Z_3 \sim \mathcal{TN}_c(0, 1)$ and $\widetilde{\mathbf{Y}}_3 \sim \mathcal{N}_d(\mathbf{0}_d, I_d)$, the convolution representation of ESN random vectors conducts to an additional identification problem that arises when Ω is "large" or "small" compared to $\mathbf{d}$—more variability of one of the convolution-based density is at the expense of weak identification of the other convolution-based density. In this respect, we assume that $\mathbf{d}|(\boldsymbol{\xi}, \Omega) \sim \mathcal{N}_d(\boldsymbol{\mu}_{\mathbf{d}}, \frac{\Omega}{\kappa_{\mathbf{d}}})$ where $\kappa_{\boldsymbol{d}} = \frac{2}{\sigma^2_{\alpha}(\tilde{\nu}-d-1)}$ yielding, in average, the same variance for both $\mathbf{d}$ and $\boldsymbol{\alpha}$. The

choice of a Gaussian distribution for $(\mathbf{d}|\Omega)$ is motivated by the fact that, together with the assumption that the prior distribution of $(\boldsymbol{\xi}, \Omega)$ is the normal-inverse Wishart distribution $\pi(\boldsymbol{\xi}, \Sigma|\tilde{\boldsymbol{\xi}}_0, \tilde{\kappa}, \tilde{\nu}, \tilde{V})$, we can easily implement a Gibbs sampler when c is known (Sahu et al., 2003). Say differently, the Gaussian prior for $\mathbf{d}$ and the normal-inverse Wishart prior for $(\boldsymbol{\xi}, \Omega)$ are the natural choice for the SN distribution of Sahu et al. (2003). Since $\Sigma - \Omega = \frac{\Sigma \boldsymbol{\alpha}\boldsymbol{\alpha}'\Sigma}{c_0^2}$, which is a positive definite matrix, we take $(\tilde{\nu}, \tilde{V})$ such that the inverse Wishart distribution $\mathcal{W}^{-1}(\tilde{V}, \tilde{\nu})$ gives more weight to "small" values than the $\mathcal{W}^{-1}(V, \nu)$ distribution. One way to capture this idea is to take $\tilde{V}$ such that $V - \tilde{V}$ is positive definite and $\tilde{\nu} \geq \nu$. Under this setting, the difference between the mode under $(\tilde{\nu}, \tilde{V})$ and the mode under (ν, V) is negative definite. This also holds for the mean.

4.3.3 A tempering SMC sampler for multivariate ESN distributions

Following Del Moral et al. (2006), our tempered SMC sampler consists in building a sequence of (initial and intermediate) distributions $\{\pi_t(\mathrm{d}\theta)\}_{t=1}^T$, assigning importance weights, resampling and moving the system.

Initial and intermediate sequence of distributions From a theoretical point of view, one can use any distribution η_1 such that $\pi_1 \ll \eta_1$. At the same time, the choice of the initial distribution might be critical for the speed of convergence of the algorithm and for the precision of the estimates. The first obvious option is to take the prior distribution, so that the SMC sampler moves simulations from the prior to simulations from the posterior distribution. Nevertheless, starting the SMC sampler with simulations from the prior can lead to very low convergence rate of the algorithm and large Monte-Carlo error since there is no reason for the prior to be closed to the posterior. A better approach consists in initializing the sampler with an approximation of the target distribution from which we can easily sample. When we are able to maximize the posterior distribution, this is effectively done by a Laplace approximation. In this case, $\eta_1(\mathrm{d}\theta)$ would be a normal distribution with mean $\mathbf{m}_1$ and covariance matrix Σ_1, with $\mathbf{m}_1$ the mode of the posterior and Σ_1 equals to minus the inverse of the Hessian matrix evaluated at this point. In some settings (see Section 4.4), the numerical maximization of the posterior distribution is particularly troublesome. In this case, we use a pilot run of a Gaussian random walk Metropolis-Hastings algorithm to get an estimate $\hat{\mathbf{m}}$ of the posterior mean and an estimate $\hat{\Sigma}$ of the posterior covariance matrix, and we define $\eta_1(\mathrm{d}\theta)$ as the a normal distribution with mean $\hat{\mathbf{m}}$ and covariance matrix $\hat{\Sigma}$.

On the other hand, the smooth sequence of intermediary distributions is purely instrumental and is defined by making use of an appropriate real sequence of so-called temperatures $\{\rho_t\}_{t=1}^T$ increasing from zero to one. According to Gelman and

Meng (1998), Neal (2001) and the tempered SMC sampler of Del Moral et al. (2006), we consider the geometric bridge:

$$\pi_t :\propto \eta_1^{1-\rho_t}\pi^{\rho_t}.$$

After defining the importance weights, we explain, in the next step, a procedure to get a suitable sequence of temperatures.

Importance weights Suppose that one has at hand a weighted sample of size N from π_{t-1}. The empirical distribution is roughly approximated by:

$$\pi_t(\theta) \approx \sum_{m=1}^{N} W_t^m(\rho_t)\delta_{\theta_t^m}(\theta)$$

where the corresponding importance function W_t is defined to be:

$$W_t^m(\rho) = \frac{w_t^m(\rho)}{\sum_{j=1}^N w_t^j(\rho)}, \qquad w_t^m(\rho) = \left[\frac{\pi(\theta_{t-1}^m)}{\pi_1(\theta_{t-1}^m)}\right]^{\rho-\rho_{t-1}}.$$

Note that $\rho_t - \rho_{t-1}$ measures the step length at time t—the larger the difference, the more the accuracy of the importance weighting worsens. To control such a degeneracy, we consider a procedure to determine a suitable sequence of $\{\rho_t\}_{t=1}^T$ through the effective sample size criterion. More specifically, instead of regarding T and the set $\{\rho_t\}_{t=1}^T$ as parameters of the algorithm, we view them as self-tuning parameters using the method proposed by Schäfer and Chopin (2012). Given a value of ρ_t and a weighted sample $\{(W_t^m, \theta_t^m)\}_{m=1}^N$ that approximates π_t, we compute the largest value of $\rho \in (\rho_t, 1]$ such that the particle system $\{\theta_t^m\}_{m=1}^N$, once being properly weighted, allows to approximate "reasonably well" the probability distribution $\pi_\rho \propto \eta_1^{1-\rho}\pi^\rho$ through the effective sample size criterion (Liu and Chen, 1995):[14]

$$\mathrm{ESS}_t(\rho) = \left[\sum_{m=1}^{N} W_t^m(\rho)^2\right]^{-1},$$

where, by definition, $W_t^m(\rho)$ is the weight assigned to θ_t^m to target π_ρ. If the effective sample size equals N, the interpretation is that the weights are equally balanced and that all N particles are equally contributing to the estimation. Then, ρ_t is defined as the minimum between 1 and $\rho_t^\star$ with

$$\rho_t^\star = \sup\{\rho > \rho_{t-1} : \mathrm{ESS}_t(\rho) \geq \beta\}$$

where β is a prespecified threshold, say $\beta = N/2$. The fixed value $\rho_t^\star$ can be obtained by solving the equation $\mathrm{ESS}_t(\rho) = \beta$ using the bi-sectional search algorithm of Schäfer and Chopin (2012) (see Algorithm 4.2).

[14]Other criteria could be the coefficient of variation of Kong et al. (1994) and the Shannon entropy of the weights. Branching algorithms could also be considered in our framework (Del Moral and Miclo, 2000).

Resampling At every ρ_t, a resampling step, using the systematic resampling method of Carpenter et al. (1999), is first performed in order to "kill" particles that are in the region of the parameter space that receives very little mass from π_t.[15] Say differently, the particles with the largest weights have multiplied whereas those with the smallest weights have vanished after the resampling step. Note that, in the absence of a proper propagation step, repeating the weighting and resampling steps will lead to the undesirable situation in which only few particles survive.

Propagation Then, at iteration $t > 1$, particle diversity is restored by moving the resampled particles by use of a Markov Kernel $K_t^N(\theta', \mathrm{d}\theta)$ having π_t as invariant distribution. More precisely, we take for $K_t^N(\theta', \mathrm{d}\theta)$ the Markov kernel that corresponds to τ steps of the Gaussian random-walk Metropolis-Hastings algorithm with variance-covariance matrix given by $c_s\Omega_t^N$, where c_s is a scale factor such that the acceptance rate of the kernel lies in the range $[0.2, 0.6]$ and where Ω_t^N is a particle based estimation of the variance-covariance matrix that corresponds to the distribution π_t.

At the end of each iteration, $\pi_\rho(\theta)$ can be defined for both parameterizations as follows.

$$\begin{aligned}
\pi_\rho(\theta) &\propto \left[\phi_d\left(\theta, \mathbf{m}_1, \Sigma_1\right)\right]^{1-\rho} \\
&\quad \times \left[\pi_{P1}(\theta) \prod_{i=1}^{n} \phi_d\left(\mathbf{z}_i, \boldsymbol{\xi}, \Sigma\right) \frac{\Phi(\lambda + \boldsymbol{\alpha}'(\mathbf{z}_i - \boldsymbol{\xi}))}{\Phi\left(\lambda/c_0\right)}\right]^{\rho} \\
w_t(\rho,\, \theta) &= \left[\phi_d\left(\theta, \mathbf{m}_1, \Sigma_1\right)\right]^{\rho_{t-1}-\rho} \\
&\quad \times \left[\pi_{P1}(\theta) \prod_{i=1}^{n} \phi_d\left(\mathbf{z}_i, \boldsymbol{\xi}, \Sigma\right) \frac{\Phi(\lambda + \boldsymbol{\alpha}'(\mathbf{z}_i - \boldsymbol{\xi}))}{\Phi\left(\lambda/c_0\right)}\right]^{\rho-\rho_{t-1}}.
\end{aligned}$$

while, under P2,

$$\begin{aligned}
\pi_\rho(\theta) &\propto \left[\phi_d\left(\theta, \mathbf{m}_1, \Sigma_1\right)\right]^{1-\rho} \\
&\quad \times \left[\pi_{\mathrm{P1}}(\theta) \prod_{i=1}^{n} \phi_d\left(\mathbf{z}_i, \boldsymbol{\xi}, \Omega + \mathbf{d}\mathbf{d}'\right) \frac{\Phi\left(c_0\left\{c + \mathbf{d}'\left[\Omega + \mathbf{d}\mathbf{d}'\right]^{-1}\left(\mathbf{z}_i - \boldsymbol{\xi}\right)\right\}\right)}{\Phi\left(c\right)}\right]^{\rho} \\
w_t(\rho,\, \theta) &= \left[\phi_d\left(\theta, \mathbf{m}_1, \Sigma_1\right)\right]^{\rho_{t-1}-\rho} \\
&\quad \times \left[\pi_{\mathrm{P2}}(\theta) \prod_{i=1}^{n} \phi_d\left(\mathbf{z}_i, \boldsymbol{\xi}, \Omega + \mathbf{d}\mathbf{d}'\right) \frac{\Phi\left(c_0\left\{c + \mathbf{d}'\left[\Omega + \mathbf{d}\mathbf{d}'\right]^{-1}\left(\mathbf{z}_i - \boldsymbol{\xi}\right)\right\}\right)}{\Phi\left(c\right)}\right]^{\rho-\rho_{t-1}}
\end{aligned}$$

where $c_0 = \left[1 - \mathbf{d}'\left[\Omega + \mathbf{d}\mathbf{d}'\right]^{-1}\mathbf{d}\right]^{-1/2}$.

[15] Alternatives approaches consist in applying a multinomial resampling (Gordon et al., 1993) or a stratified resampling (Kitagawa, 1996).

Finally we summarize the complete tempered sequential Monte Carlo method in Algorithm 4.1. Any operation involving the superscript m (respectively, subscript t) must be understood as performed for $m \in 1:N$ (respectively, $t \in 0:T$) where N (respectively, T) is the total number of particles (respectively, number of iterations). Note that n denotes the sample size. In addition, the procedure to find the step length is described in Algorithm 4.2.

Algorithm 4.1 Tempering Sequential Monte Carlo Sampler

Operations must be performed for all $m = 1, \ldots, N$.
Initialization
Set $t = 2$ and $\rho_1 = 0$.
Generate $\theta_1^m \sim \eta_1(\mathrm{d}\theta)$ and compute $W^m(\rho_1)$.
while $\rho_{t-1} < 1$ **do**
Compute ρ_t using Algorithm 4.2 with inputs ρ_{t-1} and $\{\theta_{t-1}^m\}_{m=1}^N$.
Resampling: Generate $a_{t-1}^m = F_{t,N}^{-1}(u_t^m)$ where $u_t^m = \frac{m-1+u_t}{N}$, $u_t \sim \mathcal{U}((0,1))$ and

$$F_{t,N}(i) = \sum_{m=1}^{N} W^m(\rho_t)\mathbb{I}(m \leq i).$$

Propagation: Generate $\theta_t^m \sim K_t^N(\theta_{t-1}^{a_{t-1}^m}, \mathrm{d}\theta)$.
Set $t \leftarrow t + 1$.
end while

Algorithm 4.2 Find step length using Schäfer and Chopin (2012)

Input: ϵ, ρ, $\{\theta^m\}_{m=1}^N$.
$l \leftarrow 0$, $u \leftarrow 1.05$, $\delta \leftarrow 0.05$.
while $|u - l| \geq \epsilon$ and $l \leq 1 - \rho$ **do**
if $\left[\sum_{m=1}^N W^m(\rho + \delta)^2\right]^{-1} < N/2$ **then**
$u \leftarrow \delta$, $\delta \leftarrow (\delta + l)/2$
else
$l \leftarrow \delta$, $\delta \leftarrow (\delta + u)/2$
end if
end while
Return $\min(\rho + a, 1)$.

4.3.4 Discussion

Normalizing constants Using Algorithm 4.1, one can obtain estimates of the target distributions and the normalizing constants directly from the variables generated by the sampler. At time T an approximation of the target distribution π_T is

given by

$$\pi_T^N(\mathrm{d}\theta) = \sum_{m=1}^{N} W_T^m \delta_{\theta_T^m}(\mathrm{d}\theta).$$

Moreover an estimate of the normalizing constant Z_T of π_T can be obtained from the following estimate of Z_T/Z_1 (Del Moral et al., 2006):

$$\widehat{\frac{Z_T}{Z_1}} = \prod_{t=2}^{T} \widehat{\frac{Z_t}{Z_{t-1}}}, \quad \widehat{\frac{Z_t}{Z_{t-1}}} = \sum_{m=1}^{N} W_{t-1}^m(\rho_{t-1}) \frac{\pi_t(\theta_{t-1}^m)}{\pi_{t-1}(\theta_{t-1}^m)}.$$

Model selection A question of particular interest is whether the SN or the Gaussian distributions are more appropriate than the ESN distribution. Testing the ESN distribution against the SN distribution can be done using the evidence or Bayes factor between the two specification since the ESN distribution is a regular model (conditionally to the fact that $\boldsymbol{\alpha} \neq \mathbf{0}_d$). More specifically, consider the general test $H_0 : \theta = \theta^0$ against $H_1 : \theta \neq \theta^0$ where θ^0 is the vector of parameters under the null hypothesis. The evidence, denoted B_{10}, is defined to be

$$B_{10} = \frac{m_1(\mathbf{z}_{1:n})}{m_0(\mathbf{z}_{1:n})}$$

where $\mathbf{z}_{1:n}$ is the observations and $m_i(\mathbf{z}_{1:n}) = \int f_i(\mathbf{z}_{1:n}|\theta)\pi_i(\mathrm{d}\theta)$ with $f_i(\mathbf{z}_{1:n}|\theta)$ and $\pi_i(\mathrm{d}\theta)$ respectively the likelihood and the prior distribution under H_i, $i \in \{0, 1\}$.

Testing the ESN distribution against the normal distribution is more problematic. Indeed, as discussed in Section 4.2.2, if we wrongly assume that data are generated by some ESN distributions when the true underlying model is Gaussian, then the Fisher information matrix is singular and the Bayes factor might no longer be a consistent criterion to discriminate between the two competing models. More specifically, in the presence of rank deficiency of the Fisher information matrix, there are no general results regarding the Bayes factor consistency (Morin et al., 2013) and results are mostly model-dependent. We leave this issue for further research and assess the Bayes factor reliability through Monte Carlo simulations in Section 4.4. In so doing, the derivation of the Bayes factor is made simple by the application of the Gaussian conjugate prior (4.79) for $\boldsymbol{\xi}$ and Σ. Under the normality assumption, the marginal density of the observations has a known expression, given by (see e.g. Gelman et al., 2004)

$$m_0(\mathbf{z}_{1:n}) = \frac{1}{\pi^{nd/2}} \frac{\Gamma_d(\nu_n/2)}{\Gamma_d(\nu/2)} \frac{|V|^{\nu/2}}{|V_n|^{\nu_n/2}} \left(\frac{\kappa}{\kappa_n}\right)^{d/2}$$

where

$$\kappa_n = \kappa + n, \quad \nu_n = \nu + n, \quad V_n = V + \sum_{i=1}^{n} (\mathbf{z}_i - \bar{\mathbf{z}}_n)(\mathbf{z}_i - \bar{\mathbf{z}}_n)^t + \frac{\kappa n}{\kappa + n} (\bar{\mathbf{z}}_n - \boldsymbol{\xi}^0)(\bar{\mathbf{z}}_n - \boldsymbol{\xi}^0)'.$$

Taking Algorithm 4.1, the marginal density of the observations for the ESN distribution is obtained and the Bayes factor follows.

Extension One key feature of SMC algorithms is their flexibility. Notably, the implementation of Algorithm 4.1 only requires to be able to evaluate the likelihood function. The Bayesian methodology developed in this section can therefore be trivially modified to carry out parameter inference in (complicated) parametric models based on the ESN distribution. This point is illustrated in Section 4.4.2 where we apply the proposed methodology on am ESM sample selection model.

4.4 Numerical study

In this section we provide some Monte Carlo simulations in order to assess the performances of Algorithm 4.1 and the behaviour of the posterior distribution. We consider two main data generating process: (1) IID univariate extended skew-normal random variables, and (2) an extended skew-normal sample selection model (ESNSM). For the IID setting, the SMC sampler is initialized with a Laplace approximation of the posterior distribution while, for the ESNSM, the maximization of the posterior distribution turns out to be too sensitive to the choice of the initial values to build a good approximation of the posterior distribution. In that case, and as described above, we calibrate the initial distribution of the sampler using 10 000 iterations of a pilot Metropolis-Hastings algorithm. Finally, in all the simulations presented below, the propagation step of the tempered sequential Monte Carlo algorithm is based on $\tau = 3$ iterations of the Gaussian random walk Metropolis-Hastings kernel described in Section 4.3.3.

4.4.1 IID univariate ESN random variables

We first consider a sample of IID ESN random variables. To study the implications of the parametrization, two data generating processes are considered:

$$Z_1, \cdots, Z_n \sim \mathcal{ESN}_1(\xi = 2,\, \sigma^2 = 6,\, \alpha = 5,\, \lambda = -2) \tag{4.80}$$

and

$$Z_1, \cdots, Z_n \sim \mathcal{ESN}_1(\xi = 2,\, \omega^2 = 1,\, d = 5,\, c = -0.8) \tag{4.81}$$

where the sample size n is alternatively 1 000, 5 000, and 10 000. In the case of the parametrization P1 (respectively, P2), the variance, skewness and kurtosis are respectively given by 2, 1 and 4 (respectively, 6.60, 0.99, and 4.28). The parameters for the prior distributions defined in Section 4.3.2 we use in this numerical study are $\kappa = 0.1$, $\boldsymbol{\mu}_{\boldsymbol{\alpha}} = \boldsymbol{\mu}_{\mathbf{d}} = \boldsymbol{\xi}_0 = \mathbf{0}$, $\nu = \max(6, d+4)$, $V = 12 I_d$, $\tilde{V} = 2 I_d$, $\tilde{\nu} = \nu$, $\tilde{\boldsymbol{\xi}}_0 = \boldsymbol{\xi}_0$, $\tilde{\kappa} = \kappa$ and $\sigma^2_{\boldsymbol{\alpha}} = 10$.

Parameters estimation Tables 4.1 and 4.2 report respectively the results for the $\mathcal{ESN}_1$ distributions (4.80) and (4.81) when the sample size is 1 000 and 5 000. Several points are worth commenting. First, the parametrization matters irrespective of the posterior statistics criterion used to compare the overall fitting (posterior mean, posterior median or posterior mode) and of the sample size. More specially, when the true model is defined from P1, the posterior mean, median or mode using the second parametrization depict a non-negligible bias. In contrast, when the true model is defined from P2, the discrepancy between the posterior statistics is reduced. This is clearly illustrated in the first and in the last columns of Figure 4.1 which display the marginal posterior distributions using P1 and P2 when the sample size is 1 000.

	Estimation under P1			Estimation under P2		
	Mean	Median	Mode	Mean	Median	Mode
$\xi = 2$	1.70	1.74	1.77	0.53	0.54	0.56
	(0.010)	(0.009)	(0.012)	(0.008)	(0.009)	(0.012)
	1.84	1.85	1.86	1.38	1.39	1.40
	(0.002)	(0.003)	(0.005)	(0.003)	(0.004)	(0.006)
$\sigma^2 = 6$	5.86	5.79	5.74	7.52	7.48	7.45
	(0.017)	(0.016)	(0.019)	(0.011)	(0.013)	(0.016)
	6.22	6.20	6.19	6.93	6.92	6.91
	(0.004)	(0.005)	(0.009)	(0.005)	(0.006)	(0.010)
$\alpha = 5$	4.01	3.99	3.98	3.04	3.01	3.00
	(0.006)	(0.006)	(0.010)	(0.006)	(0.005)	(0.007)
	4.71	4.70	4.69	4.03	4.02	4.02
	(0.003)	(0.004)	(0.006)	(0.002)	(0.003)	(0.005)
$\lambda = -2$	-3.10	-2.94	-2.84	-6.24	-6.15	-6.08
	(0.040)	(0.036)	(0.041)	(0.023)	(0.024)	(0.029)
	-2.76	-2.71	-2.68	-4.36	-4.33	-4.30
	(0.011)	(0.014)	(0.021)	(0.011)	(0.013)	(0.022)
$\log m(z_{1:n})$		-1 473.84			-1 532.98	
		(38.37)			(34.00)	
		-8 065.57			-8 074.10	
		(13.01)			(18.22)	
time (in seconds)		60.22			34.05	
		120.44			124.26	

Table 4.1: Estimation of univariate $\mathcal{ESN}_1$ distributions (4.80). The results are obtained from 50 estimations of the model with $N = 10\,000$ particles. The mean values are reported and the standard deviations are given in bracket. For each parameter, the first two lines are for n =1 000 and the last two lines are for n =5 000.

	Estimation under P1			Estimation under P2		
	Mean	Median	Mode	Mean	Median	Mode
$\xi = 2$	3.52	3.66	3.77	1.79	1.82	1.86
	(0.031)	(0.030)	(0.035)	(0.017)	(0.019)	(0.029)
	3.01	3.07	3.11	2.52	2.54	2.56
	(0.010)	(0.012)	(0.022)	(0.010)	(0.010)	(0.014)
$\sigma^2 = 26$	22.71	22.34	22.04	27.76	27.55	27.40
	(0.092)	(0.082)	(0.094)	(0.045)	(0.051)	(0.071)
	24.86	24.71	24.58	26.28	26.21	26.15
	(0.029)	(0.037)	(0.055)	(0.024)	(0.030)	(0.046)
$\alpha = 0.98$	1.00	1.00	1.00	1.00	0.96	0.98
	(0.001)	(0.001)	(0.001)	(0.001)	(0.001)	(0.002)
	1.01	1.02	1.01	1.01	1.01	1.01
	(0.000)	(0.000)	(0.001)	(0.001)	(0.000)	(0.001)
$\lambda = -4.08$	-2.44	-2.32	-2.21	-4.33	-4.26	-4.21
	(0.032)	(0.031)	(0.034)	(0.019)	(0.019)	(0.033)
	-3.05	-3.00	-2.96	-3.57	-3.55	-3.54
	(0.010)	(0.013)	(0.021)	(0.009)	(0.010)	(0.018)
$\log m(z_{1:n})$	-2 244.49			-2 184.73		
	(41.69)			(30.01)		
	-11 500.13			-11 476.46		
	(25.22)			(41.65)		
time (in seconds)	38.52			61.40		
	125.98			165.89		

Table 4.2: Estimation of univariate $\mathcal{ESN}_1$ distributions (4.81). The results are obtained from 50 estimations of the model with $N = 10\,000$ particles. The mean values are reported and the standard deviations are given in bracket. For each parameter, the first two lines are for $n = 1\,000$ and the last two lines are for $n = 5\,000$.

Second, Table 4.1 and Figure 4.1 provide evidence that the P1-posterior modes are rather close to the true parameters of the ESN distribution when the true distribution is defined by P1, with the main exception of the α parameter. Note that the posterior mean and the posterior model may display some important differences due to the asymmetry of the posterior distributions. On the other hand, the P2-posterior statistics have a significant bias. Looking at the Bayes factor, one see (as expected) a clear evidence in favour of the results obtained under P1. Assuming that the true distribution is defined from P2, we now logically observe better results for the estimates obtained under this parametrization than for those computed under P1 (as underlined by the Bayes factor which is now in favour of P2). However, the P1-posterior mode leads to fairly closed values to the true parameters (expect for the location parameter ξ).

To explain the poor estimations obtained under P2 for the $\mathcal{ESN}_1$ distribution (4.80), note that in this case the parameters are such that ω^2 is close to the boundary of the parameter space ($\omega^2 \approx 0.038$). Hence, inference for this parameter is very sensitive to the choice of the prior distribution (see e.g. Newton and Raftery, 1994; Gelman, 2006). In particular, the prior we choose for ω^2 puts very small weight to values close to zero and therefore tends to overestimate ω^2. This problem of

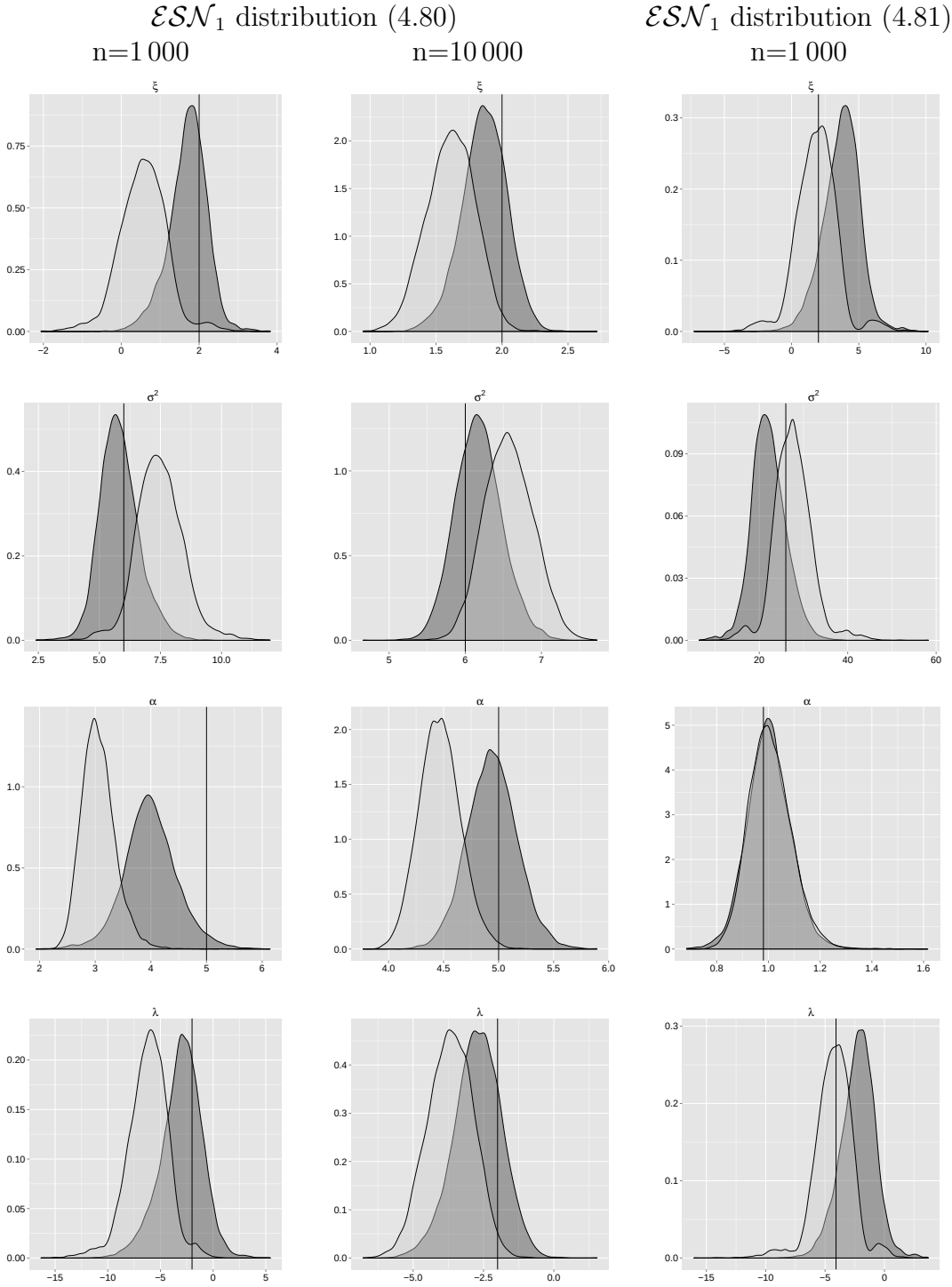

Figure 4.1: Marginal posterior distributions for the parameters of the $\mathcal{ESN}_1$ distributions (4.80) and (4.81). Results for P1 (respectively, P2) are in dark (respectively, in grey) and are obtained for $N = 10\,000$.

	(α, λ)	$\log_{10} B_{10} \leq 0.5$	$0.5 < \log_{10} B_{10} \leq 1$	$1 < \log_{10} B_{10} \leq 2$	$\log_{10} B_{10} > 2$
n=100	(0,-)	100%	0%	0%	0%
	(5,-2)	1%	1%	4%	96%
	(0.5,1)	100%	0%	0%	0%
n=5 000	(0.5,1)	0%	0%	0%	100%

Table 4.3: Bayes factors. The results are obtained from 100 samples. The number of particles is 10 000 and B_{10} denotes the Bayes factor to test the normality hypothesis.

parameters close to the boundary is particularly serious because even "non informative" prior distributions can have a big effect on inference (see e.g. Gelman et al., 2008). For that reason, and contrary to the current practise (see e.g. Adock, 2004; Liseo and Parisi, 2013), we advocate for the use of the $(\boldsymbol{\xi}, \Sigma, \boldsymbol{\alpha}, \lambda)$-parametrization to carry out parameter inference in the ESN (and in the SN) distribution.

However, and this is our third observation, when the sample size gets larger and larger, the posterior modes converge toward the true values of the parameters irrespective of the chosen parametrization. In particular, the middle column of Figure 4.1 provides strong support for the convergence of the marginal posterior modes when the sample size is 10 000.

Finally, taking the low number of particles ($N = 10\,000$), the Monte Carlo error is rather small in all cases and for all parameters, especially as the sample size increases. However, it is at the expense of a somehow large computing time which is, under both parametrization, around 90 seconds for $n = 1\,000$ and around 460 seconds for $n = 5\,000$.

Model selection As explained in Section 4.3.4, it is critical to assess the robustness of ESN distributions with respect to Gaussian distributions. In this respect, we conduct some simulation experiments regarding the Bayes factor using univariate extended skew-normal random variables—the investigation of the specification tests for the bivariate extended skew-normal random vectors leads to the same results. Therefore we test the null hypothesis of normality against the alternative hypothesis of an extended skew-normal distribution, $\mathcal{ESN}_1(2, 6, \alpha, \lambda)$ for different (α, λ) pairs, and some selected results are reported in Table 4.3. According to the terminology of Jeffreys (1939), Table 4.3 shows the percentage of sample where the evidence in favour of the ESN hypothesis is poor ($\log_{10} B_{10} \leq 0.5$), substantial ($0.5 < \log_{10} B_{10} \leq 1$), strong ($1 < \log_{10} B_{10} \leq 2$) and decisive ($\log_{10} B_{10} > 2$). The results reported in the first three lines of Table 4.3 are obtained for a sample size of $n = 100$. We observe that, despite the small number of observations, the Bayes factor yields very good results for $(\alpha, \lambda) = (0, -)$ (i.e., Gaussian model) and $(\alpha, \lambda) = (5, -2)$. Indeed, in both cases and in all samples, the Bayes factor selects the correct model with a strong confidence. For $(\alpha, \lambda) = (0.5, 0)$, estimations are in favour of the Gaussian distribution although the underlying model is ESN. This

results is intuitive. Indeed, the Bayes factor penalizes for the number of parameters. Therefore, since λ is useless when the underlying model is Gaussian, it is natural that the Bayes factor is biased toward the Gaussian distribution when α is close to zero. In contrast, when the sample size increases (from $n = 100$ to $5\,000$), the Bayes factor selects the correct model with a strong confidence. These results suggest that the Bayes factor is convergent even if no formal proof for this specific test is yet available in the literature (see Section 4.3.4).

4.4.2 Extended skew-normal sample selection model

Thanks to Definition 4.1, the application of ESN distribution in sample selection models or Tobit-type models (Amemiya, 1986; Maddala and Lee, 1976) is a natural choice since any hidden truncation of normal component densities leads to such a distribution (see Arnold and Beaver, 2002). In this respect, starting from the Gaussian sample selection model (Heckman, 1976), a (multivariate) extended skew-normal sample selection model (ESNSM) can be defined by:

$$\begin{cases} \mathbf{Y}_i^* = B\mathbf{x}_i + \boldsymbol{\epsilon}_{1i} \\ S_i^* = \boldsymbol{\beta}_2'\mathbf{x}_i + \epsilon_{2i}, \quad i = 1, ..., n \end{cases} \tag{4.82}$$

where $B \in \mathbb{R}^{d \times k_1}$, $\boldsymbol{\beta}_2 \in \mathbb{R}^{k_1}$, and

$$\boldsymbol{\epsilon}_i \sim \mathcal{ESN}_{d+1}\left(\boldsymbol{\xi} = (\boldsymbol{\xi}_1, \xi_2), \Sigma = \begin{pmatrix} \Sigma_1 & \Sigma_{12} \\ \Sigma_{21} & 1 \end{pmatrix}, \boldsymbol{\alpha} = (\boldsymbol{\alpha}_1, \alpha_2), \lambda\right) \tag{4.83}$$

with $\boldsymbol{\xi} = -\frac{\Sigma\boldsymbol{\alpha}}{c_0}\frac{\phi(\lambda/c_0)}{\Phi(\lambda/c_0)}$ such that $\mathbb{E}[\boldsymbol{\epsilon}_i] = \mathbf{0}_d$. We assume that we observe $S_i = \mathbb{I}_{\mathbb{R}_+}(S_i^*)$ and $\mathbf{Y}_i = \mathbf{Y}_i^* S_i$ with $\mathbb{I}_A(\cdot)$ the indicator function of $A \subseteq \mathbb{R}$. The likelihood function of the model, required to compute the importance weights in the SMC sampler (Algorithm 4.1), follows from a direct application of Proposition 4.1 (closure under conditioning and marginalization of the extended skew-normal family of distributions):

$$L_n(\theta, \boldsymbol{\beta}_2, B) = \prod_{i=1}^{n} \left[\frac{\Phi_2\left(-\boldsymbol{\beta}_2'\mathbf{x}_i - \xi_2, 1, c_2\tilde{\alpha}_2, c_2\lambda\right)}{\Phi\left(\frac{c_2\lambda}{\sqrt{1+c_2^2\tilde{\alpha}_2^2}}\right)} \right]^{1-s_i}$$

$$\times \left[\phi_d\left(\mathbf{y}_i, B\mathbf{x}_i + \boldsymbol{\xi}_1, \Sigma_1\right) \frac{\Phi_2(m_i, \sigma_{22.2}^2, -\alpha_2, \lambda + \tilde{\boldsymbol{\alpha}}_1'(\mathbf{y}_i - B\mathbf{x}_i - \boldsymbol{\xi}_1))}{\Phi\left(\frac{c_1\lambda}{\sqrt{1+\tilde{\boldsymbol{\alpha}}_1'\Sigma_1\tilde{\boldsymbol{\alpha}}_1 c_1^2}}\right)} \right]^{s_i}$$

where $m_i = \boldsymbol{\xi}_1 + \boldsymbol{\beta}_2'\mathbf{x}_i + \Sigma_{12}\Sigma_1^{-1}(\mathbf{y}_i - B\mathbf{x}_i - \boldsymbol{\xi}_1)$ and with $\tilde{\alpha}_1$ and $\tilde{\boldsymbol{\alpha}}_2$ defined as in Proposition 4.1. The prior distributions for the parameters $\boldsymbol{\alpha}$ and λ are as above while those for Σ, B and $\boldsymbol{\beta}_2$ are discussed in Appendix B.

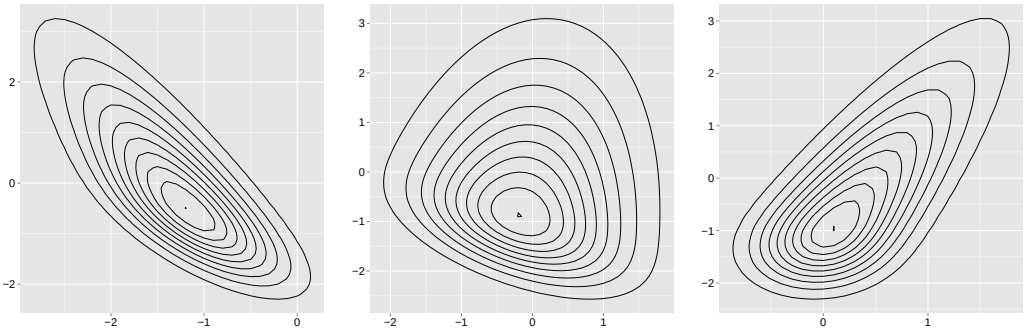

Figure 4.2: Level curves of the zero mean $\mathcal{ESN}_2$ distribution (4.85) for $\rho = -0.9$ (left plot), $\rho = 0.3$ (middle plot) and for $\rho = 0.9$.

The numerical study is conducted for the univariate extended skew-normal sample selection model

$$\begin{cases} Y_i^* = \beta_{10} + \beta_{11} x_{1i} + \epsilon_{1i} \\ S_i^* = \beta_{20} + \beta_{22} x_{2i} + \epsilon_{2i}, \end{cases} \tag{4.84}$$

and

$$(\epsilon_{1i}, \epsilon_{2i}) \sim \mathcal{ESN}_2 \left(\boldsymbol{\xi}, \left(\begin{smallmatrix} 6 & \rho\sqrt{6} \\ \rho\sqrt{6} & 1 \end{smallmatrix} \right), (2,1), -2 \right) \tag{4.85}$$

where $\rho \in \{-0.9, 0.3, -0.9\}$. The parameter value of ρ is a key issue in sample selection models. Notably when $\rho = 0$, there is no selection effect. On the other hand, it can be shown that the correlation between ϵ_{1i} and ϵ_{2i} increases with this parameter: this is clearly illustrated in Figure 4.2. The parameter values for the slope (β) parameters are respectively given by $\beta_{10} = 3$, $\beta_{11} = -2$, $\beta_{20} = 1.5$ and $\beta_{22} = 2$ while the covariates x_{1i} and x_{2i} are assumed to be independent $\mathcal{N}_1(0, 2)$ random variables (without loss of generality). This setup implies that $S_i = 0$ for about $30\% - 35\%$ of the $n = 1\,000$ observations.

We now discuss some Monte Carlo simulations results for the univariate extended skew-normal sample selection model (4.84)-(4.85) and compare it with the standard Tobit-type 2 model (i.e., the sample selection model with Gaussian errors, see Amemiya (1986)). Notably this comparison is based on the estimation of the parameters and of the marginal effects as well as a testing procedure regarding the selection effect.

Parameters estimation Table 4.4 provides the posterior mean and the standard deviation of 50 independent estimates of the parameters of the model (4.84)-(4.85) under the two alternatives parametric assumptions (i.e., the bivariate extended skew-normal and the Gaussian distribution of the error terms). Results are reported for the three different values of ρ.

Parameter	ρ	Tobit 2		ESNM		True value
		Mean	Standard deviation	Mean	Standard deviation	
β_{10}	0.3	2.92	0.0008	2.94	0.0006	3
	0.9	2.98	0.0006	2.99	0.0005	
	-0.9	2.97	0.0005	2.98	0.0006	
β_{11}	0.3	-1.98	0.0004	-1.96	0.0004	-2
	0.9	-1.99	0.0004	-1.99	0.0003	
	-0.9	-1.99	0.0003	-1.990	0.0352	
β_{20}	0.3	1.58	0.0010	1.37	0.0015	1.5
	0.9	2.57	0.0020	1.78	0.0021	
	-0.9	2.10	0.0015	1.43	0.0020	
β_{22}	0.3	2.04	0.0013	1.77	0.0020	2
	0.9	3.32	0.0026	2.30	0.0026	
	-0.9	2.77	0.0020	1.87	0.0028	
σ_1^2	0.3	2.22	0.0012	6.04	0.0101	(6)
	0.9	2.10	0.0011	5.74	0.0074	
	-0.9	1.60	0.0008	6.08	0.0113	
ρ	0.3	0.06	0.0010	0.39	0.0015	
	0.9	0.63	0.0010	0.82	0.0006	
	-0.9	-0.76	0.0008	-0.90	0.0004	
α_1	0.3	-	-	3.04	0.0154	(2)
	0.9	-	-	3.27	0.0165	
	-0.9	-	-	1.86	0.0066	
α_2	0.3	-	-	2.17	0.0145	(1)
	0.9	-	-	2.15	0.0251	
	-0.9	-	-	0.55	0.0134	
λ	0.3	-	-	-2.54	0.0234	(-2)
	0.9	-	-	-1.85	0.0207	
	-0.9	-	-	-3.38	0.0164	
$\log m(z_{1:n})$	0.3	-1 448.91	0.00251	-1 313.91	0.0269	
	0.9	-1 358.97	0.00401	-1 206.92	0.0504	
	-0.9	-1 291.19	0.0059	-1 168.48	0.0262	

Table 4.4: Estimation of sample selection model (4.84)-(4.85). The results are obtained from independent 50 independent estimations and are obtained for $N = 10\,000$.

Regarding the estimation of the constant and slope parameters of the regression equation, β_{10} and β_{11}, we observe that the distributional assumption has very few impact on the estimated values in all scenarios. A similar result is observed for the Student selection model in Marchenko and Genton (2012) and for the skew-normal model in Ogundimu and Hutton (2012). On the other hand, the estimation of the corresponding parameters in the selection equation, β_{20} and β_{22}, are more sensitive to the choice of the error terms distribution. Indeed, if the Gaussian assumption leads to a small bias for these parameters when the correlation between the variable of interest and the selection variable is low (i.e. when $\rho = 0.3$, implying a correlation between -0.02 and -0.03), the results obtained with the Tobit 2 model for these parameters are significantly biased for larger values of $|\rho|$.

To illustrate the importance of the bias for β_{20} and β_{22}, Figure 4.3 reports, for the dataset with $\rho = 0.9$, the individual estimates over 50 simulations when the error terms are misspecified—they are wrongly assumed to be normally distributed. Taking that the true parameter vector is given by $(\beta_{20}, \beta_{22}) = (1.5, 2)$, we observe that all of the estimates of β_{20} and β_{22} are much larger than the true underlying parameter values. To some extent, this result is consistent with standard results relative to the misspecification issues of the maximum likelihood estimator of Tobit-type models in the literature.

In contrast, when the model is correctly specified, the constant and slope parameters of the selection process are well-estimated irrespective of the correlation parameter ρ. Notably, the posterior mean of each parameter is close to the true parameter value and the estimation error is small. Regarding the other parameters of the model we obtain very good estimations of σ_1^2 and ρ for which we observe both a small bias and a small standard deviation. The estimation of α_2 turns out to be more complicated due to loss of information created by the censorship of S_i^*. Moreover, the posterior mean of λ is close to the true value at the expense of a relatively large standard deviation (precision), especially with respect to other parameters.

Further evidence is provided by Figure 4.4, which displays the marginal posterior distributions of the parameters in the case of one realization of the model (4.84)-(4.85) with $\rho = 0.3$. In addition to the previous results, three points are worth commenting. First, the posterior modes are close to the true parameter values. Second, the marginal distribution for the β's parameters are very concentrated around the mode. Third, the sign of the α's parameters, and hence of the skewness of the data, is well identified since the posterior mass on $\{\alpha_i < 0, i = 1, 2\}$ is close to zero. In contrast, there is a small but significant posterior probability for the event $\{\lambda > 0\}$ suggesting that more observations are needed to identify more precisely this parameter.

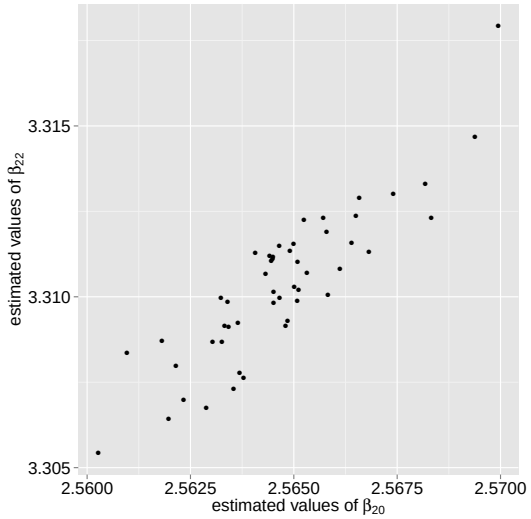

Figure 4.3: Bias for selection coefficients under Tobit type-2 model. The graph presents 50 independent estimates of the selection coefficient (β_{20}, β_{22}). The true parameter vector is $(\beta_{20}, \beta_{22}) = (1.5, 2)$ and the results are for the dataset with $\rho = 0.9$, $N = 10\,000$ particles.

Marginal effects For ease of interpretation, it is arguably better to consider the (average) marginal effects (Cameron and Trivedi, 2005) since only the sign (but not the magnitude) of the coefficients can be readily interpreted in Tobit-type models. In this respect, we compute the marginal effects (see Proposition 4.1 in Appendix B) and Figure 4.4 displays marginal effect estimates of β_{22} on $\mathbb{E}[Y_i^*|S_i = 1, \mathbf{x}_i]$ for a realization of the above model with $\rho = 0.3$. The main result is that the Gaussian model is not able to account for important heterogeneity in marginal effects. Indeed, we see that the distribution of Gaussian estimates is much more concentrated than the distribution of the true values. In addition, the marginal effects obtained from the Tobit 2 models are in all cases larger than -10 although for a lot of individuals the marginal effect of β_{22} is indeed smaller than this threshold (with a minimum nearby -60). The average effect estimate under the Gaussian assumption is around -0.14 while the true value is about 15 times larger (around -2.08). In contrast, this estimate under the ESN assumption is -2.22. The values of the marginal effects estimated under the correct parametric assumption are also reported and are, as to be expected, very close to the true values.

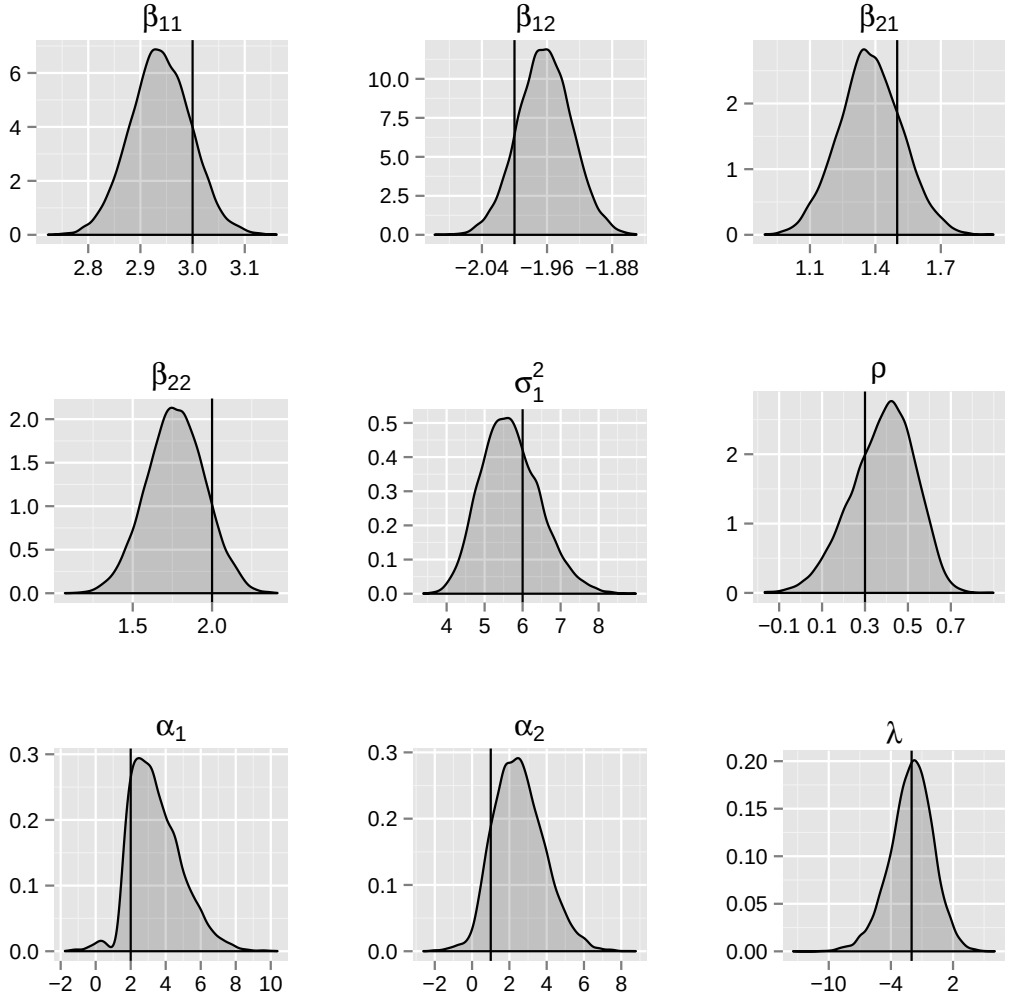

Figure 4.4: Marginal Posterior distribution of the ESNSM (4.84)-(4.85) with $\rho = 0.3$ and the marginal posterior distribution are estimated using the SMC sampler described above with 50 000 particles.

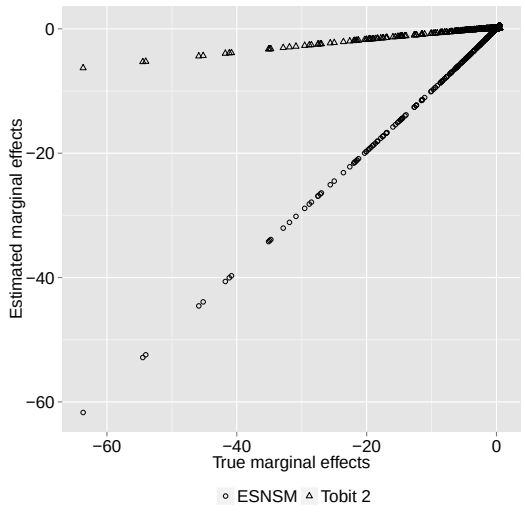

Figure 4.5: Marginal effects for the ESNSM (4.84)-(4.85) with $\rho = 0.3$. For each individual, the plot gives the marginal effects as estimated by the Tobit 2 and the ESNSM against its true value. The results are obtained for $N = 50\,000$ particles.

Sample selection effect As pointed out by Marchenko and Genton (2012) mispecifying the distribution may lead to incorrect conclusions concerning the existence of a selection effect. To illustrate this point we analyse the percentage of time the Bayes factor detects the selection effect in the model (4.84)-(4.85) under the ESN and the Gaussian assumption. The analysis is done for $\rho = 0.3$ (leading to a correlation between the disturbance terms close to zero) and for $\rho = 0.5$ (implying a correlation around 0.15). As explained above, we assume that the error terms are independent ESN random variables in the context of no selection effect.

The result obtained from 100 Monte Carlo replications are reported in Table 4.5. The ESNSM detects the presence of a selection effect in about 90% of the simulations in the two scenario. The power of this test is much lower under the wrong Gaussian assumption. When the error terms are almost uncorrelated, the Tobit 2 model detects the selection effect in about only 32% of the simulations. Note that this result was expected since, from the point of view of the Gaussian model, we are close to a situation with no selection effect. When the correlation increases the evidence in favour of the Gaussian model naturally improves but the power of the test, which is around 54%, remains quite weak.

4.5 Application

As mentioned in the introductory section, and to the best of our knowledge, all applications of the ESN distribution on real data we can found in the literature are

ρ	ESNSM	Tobit2
0.3	90%	32%
0.5	88%	45%

Table 4.5: Test for Sample selection effect. The Table gives the percentage of times the Bayes factor correctly detects the selection effect. The result are obtained from 100 estimations of the model (4.84)-(4.85) with $N = 50\,000$ particles.

done for a given value of λ under the parametrization P1 (and notably for $\lambda = 0$ so that the ESN distribution reduces to the SN distribution) or, under P2, for a given value of c. However, to demonstrate the practical interest of letting λ be a free parameter we expose below two applications of the proposed methodology on real data. The first dataset is univariate and contains football transfer records while the second dataset contains the returns of two financial assets.

For both applications, the estimations are performed using the P1-parametrization (Definition 4.1) with the prior distributions as in Section 4.4.1. The SMC sampler is initialized using a pilot run of a Gaussian random walk Metropolis-Hastings and the propagation step is based on $\tau = 3$ iterations of a Gaussian Metropolis-Hastings kernel (see Section 4.3.3).

4.5.1 Univariate ESN: Foot transfer data

We consider a dataset made of the transfer price (in log) of 1 062 footballers.

Figure 4.6 presents the marginal posterior distributions assuming both ESN and SN data. The estimated value of the marginal distribution of the data under these two specification are also provided. The first point it is worth noting is that under the ESN assumption the marginal posterior distribution for λ has most of its mass on the interval $(-\infty, -2]$. Together with the fact that the posterior distribution for α has most of its mass on $[1.2, \infty)$, this suggests that the ESN model is more appropriate that the SN model of Azzalini (1985). Indeed, using the output of the SMC sampler, we find the evidence in favour of the ESN distribution is "decisive" (in the sense of Jeffreys, 1939). Finally, Figure 4.7 compares the ESN estimate of the density function of the data with a non-parametric estimate, and one can observe that both provides very similar results.

4.5.2 Bivariate ESN: Financial Data

As a final illustration of the proposed algorithm, we proceed with a real financial data set as in Liseo and Parisi (2013). There is an impressive literature in finance that

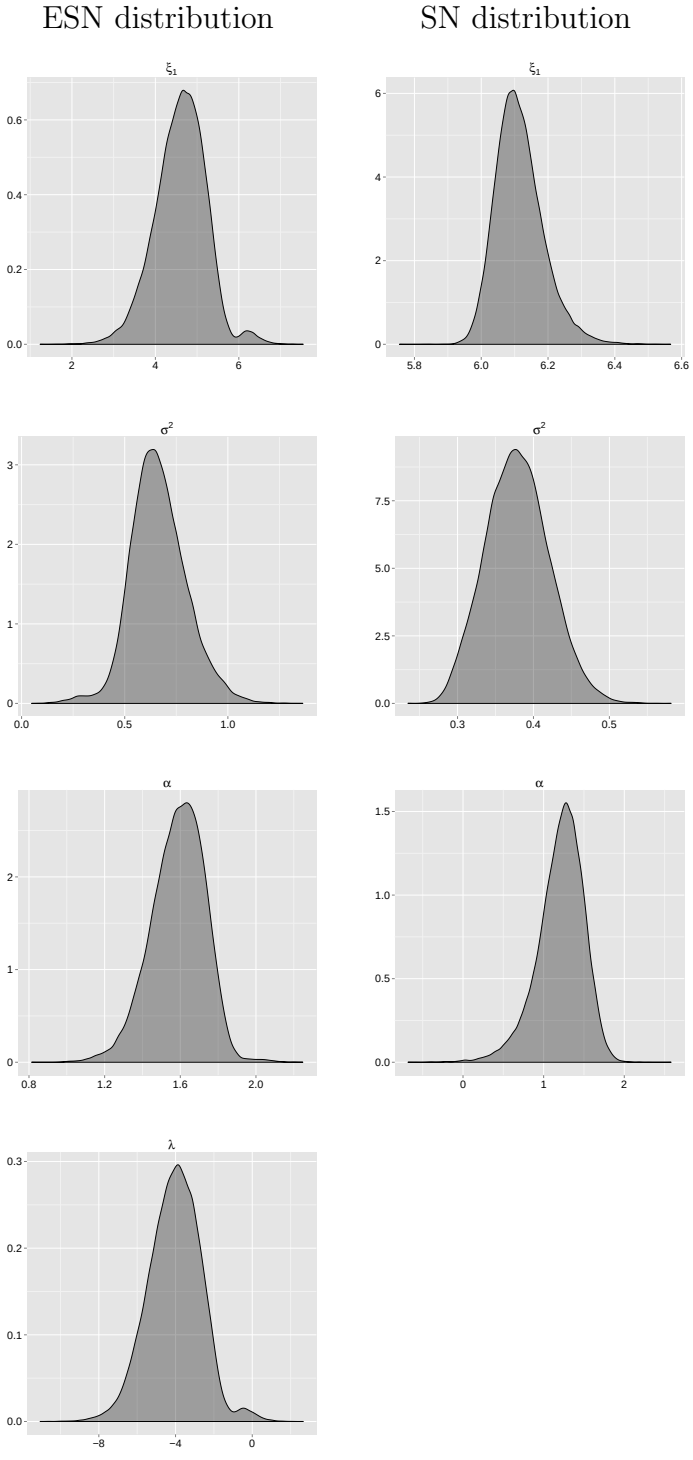

Figure 4.6: Marginal Posterior distributions for the foot transfer data. The results are obtained for $N = 50\,000$ particles. Evidence (in log) in favour of the ESN distribution is -685.0374 against -797.1437 for the SN distribution.

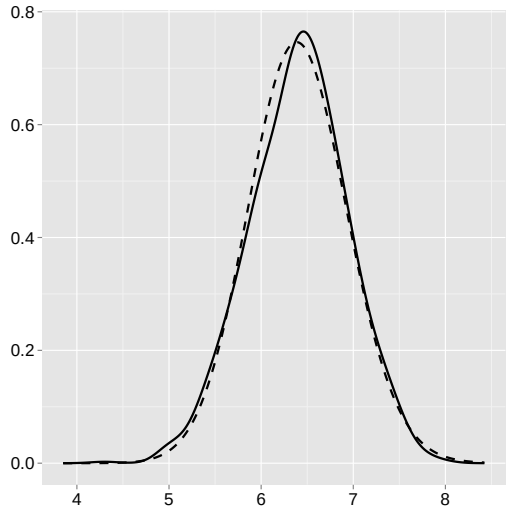

Figure 4.7: Density of the football transfer data. ESN estimate (dashed line) and non-parametric estimate (solid line). The ESN estimate is obtained with $N = 50\,000$ particles.

has witnessed the fact that (high-frequency) financial returns are skewed and display leptokurtic tails (e.g., see Jondeau et al., 2006; Genton, 2004) and may have strong implications in portfolio selection, asset pricing models or risk measurement (among others). In this respect, we consider a simple `i.i.d.` bivariate sampling model. More specifically, we analyse the weekly returns (in percentage) of two US stocks, namely "ABM Industries Incorporated" (ABM) and "The Boeing Company" (BA). The sample size covers the period Jul 19, 1984 to Jul 28, 2014 (1 566 observations).[16]

Figure 4.8 displays the raw data and the estimated $\mathcal{ESN}_2$ density whereas Figures 4.9 and Figure 4.10 depict, respectively, the marginal posterior distribution of each parameter under the ESN and the SN assumption. Two points are worth commenting. First the contour plot of the density of the estimated $\mathcal{ESN}_2$ model suggests that raw data, which are skewed and fat-tailed, can be reasonably well-captured by this specification. Second, the marginal posterior modes of the shape (α_1 and α_2) and the shift parameter (λ) are roughly given by 0.13, 0.20 and -3, respectively. Combined with the fact that the (marginal) posterior of each of these parameters has a negligible mass with positive (for λ) or negative (for α_1, α_2) values, the estimation provides strong support for the application of an extended skew-normal distribution in order to jointly model ABM and BA. Moreover, according to standard stylized financial facts of weekly returns, the location parameters, ξ_1 and ξ_2, are negative (large negative returns are more important than large positive returns) and

[16]We also perform estimation with daily and monthly returns. Our main results remain unchanged.

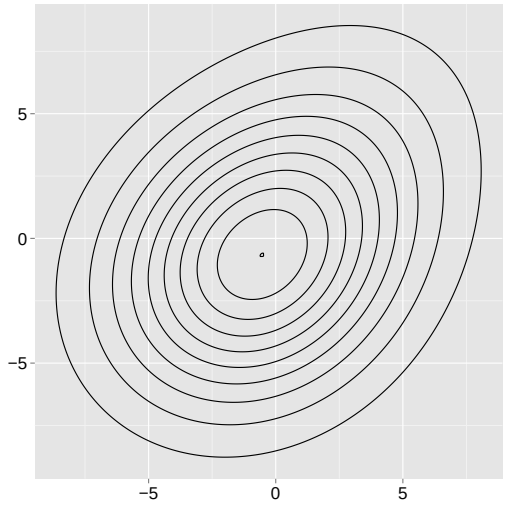

Figure 4.8: Estimated contour plot for bivariate financial data (ABM and BA)

the marginal posterior modes of the unconditional variance-covariance parameters (σ_1^2, σ_2^2, σ_{12}^2) support large volatility and co-volatility.

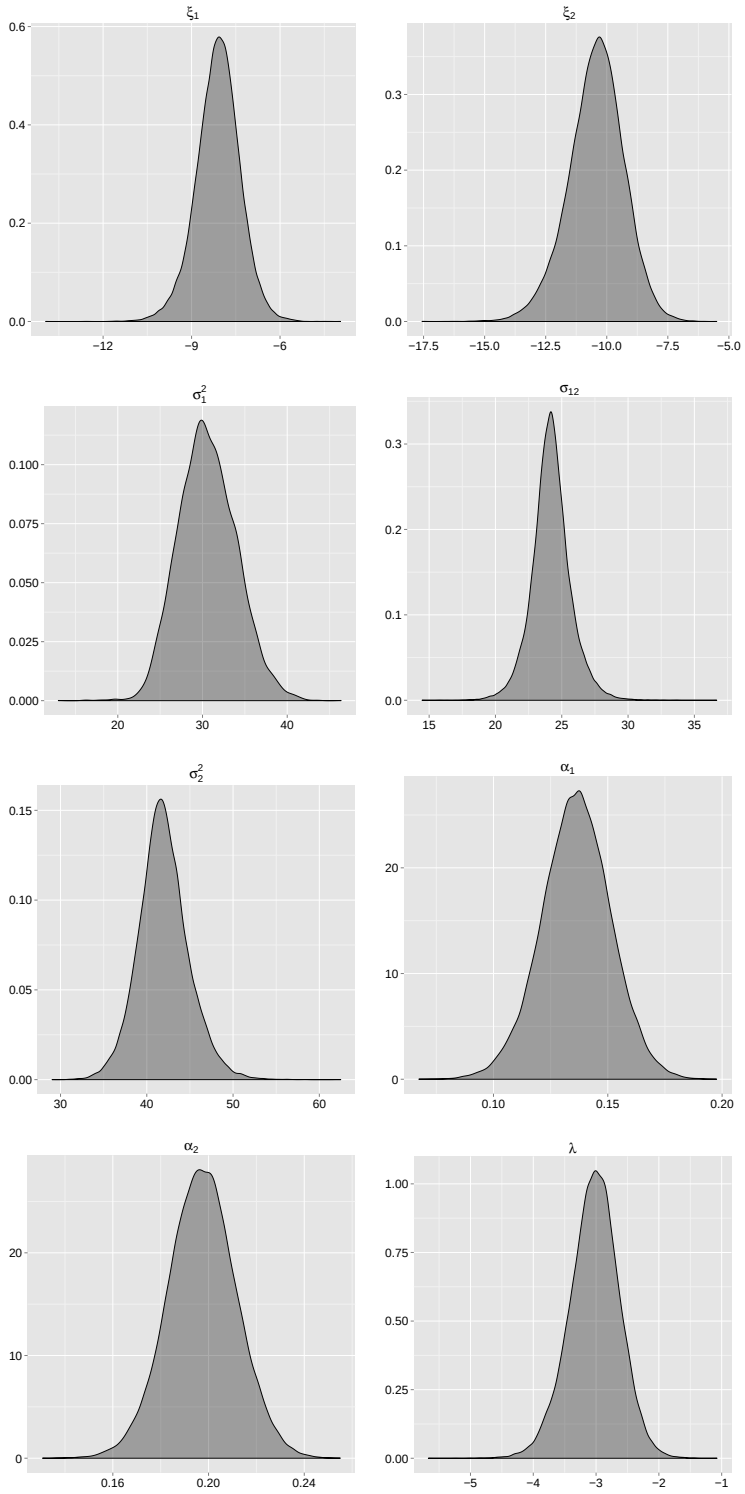

Figure 4.9: Marginal Posterior distributions for the financial data under the ESN assumption. The results are obtained for $N = 10\,000$ particles. Evidence (in log): -8 631.379.

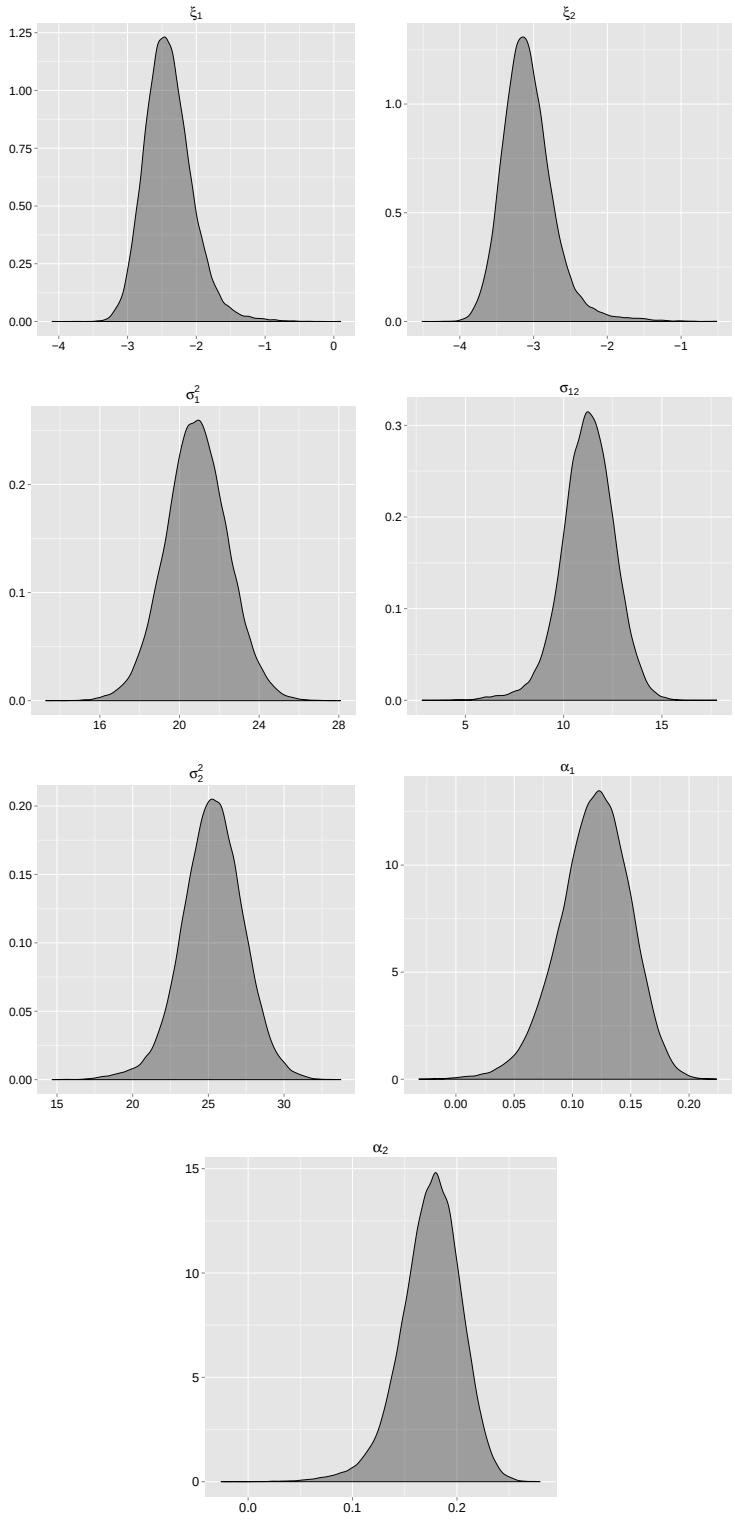

Figure 4.10: Marginal Posterior distributions for the financial data under the SN assumption. The results are obtained for $N = 50\,000$. Evidence (in log): -8 647.239.

Finally we proceed with model selection. Using the SMC estimate of the Bayes factor, we find the evidence in favour of the skew-normal bivariate distribution proposed by Liseo and Parisi (2013) is poor (in the sense of Jeffreys, 1939).

4.6 Conclusion

The (multivariate) extended skew-normal distribution allows for accommodating data which are skewed and heavy tailed while being tractable and parsimonious, and having at least three appealing statistical properties, namely closure under conditioning, affine transformations, and marginalization. Notably this class of distributions is a natural outcome in sample selection and more generally in Tobit-type models (or regressions with missing data). In this respect, we propose a new Bayesian estimation approach which rests on a tempered sequential Monte Carlo sampler.

Among others, the proposed approach have several advantages. First, it overcomes some issues encountered in standard maximum likelihood estimation. Second, in contrast to MCMC methods, it is easy to build a SMC algorithm that is adaptive in the sense that it can adjust sequentially and automatically its sampling distribution to the problem at hand provided some well-defined prior distributions. Especially, it can implemented for a large class of (multivariate) skew-elliptical distributions. Third, it allows to compute easily as a by-product the marginal posterior distributions, the normalizing constant and thus the Bayes factor. Fourth, it embeds as a special case the population algorithm provided by Liseo and Parisi (2013).

Monte Carlo simulations provide evidence regarding the robustness of the proposed algorithm with different data generating processes. Irrespective of the model considered (sampling models, extended skew-normal sample selection models), posterior statistics are rather precise (with a low standard deviation) in a tractable computing time. Moreover, the results tend to indicate that the hidden truncation-based parametrization is more robust than the convolution-based parametrization. A simple application with bivariate financial series display some interesting results for portfolio allocation, asset pricing models and risk measurements that deserve to be further analyzed. Directions for future research include more comprehensive empirical applications (Gerber and Pelgrin, 2014) and the derivation of more general models with hidden truncation, censoring or selective report with the (multivariate) extended skew-normal family of distributions or some unified skew-elliptical distributions.

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Appendix

A Proof of Proposition 4.2

Let $l_n(\theta) = \log L_n(\theta)$ and $\theta \in \Theta_\epsilon^{l^*}$ where $\Theta_\epsilon(l^*) = \{\theta : \|\theta - \theta_{n,G}^{l^*}\| \leq \epsilon\}$. Then, $l_n(\theta_{n,G}^{l^*}) - l_n(\theta) > 0$ means that

$$l_n^G(\theta_G^{l^*}) - l_n^G(\theta) - \frac{1}{N}\sum_{i=1}^{n} \log \Phi\left(l + a(z_i - m)\right) + \log \Phi(l/c_0) \geq 0$$

where l_n^G is the log-likelihood corresponding to the Gaussian model. A sufficient condition for the above inequality to hold is

$$\log \Phi\left(\frac{l^* - \epsilon}{\sqrt{1 + (\sigma_{n,G}^2 + \epsilon)\epsilon^2}}\right) \geq \log \Phi\left(l^* + \epsilon(1 + \bar{z}_n - \xi_{n,G} + \epsilon)\right)$$

where $\bar{z}_n = \max\{|z_i|\}$. This is equivalent to

$$l^* \leq l_{n,\epsilon}^* := \frac{\epsilon + \sqrt{1^* + (\sigma_{n,G}^2 + \epsilon)\epsilon^2}\,(\epsilon(1 + \bar{z}_n - \xi_{n,G} + \epsilon))}{1 - \sqrt{1^* + (\sigma_{n,G}^2 + \epsilon)\epsilon^2}}.$$

Hence, for all $\epsilon > 0$, there exists a $l_{n,\epsilon}^*$ such that

$$l^G(\theta_{n,G}^{l_{n,\epsilon}^*}) - l(\theta) - \frac{1}{N}\sum_{i=1}^{n} \log \Phi\left(l + a(z_i - m)\right) + \log \Phi(l/c_0) \geq 0 \quad \forall \theta \in \Theta_\epsilon(l_{n,\epsilon}^*).$$

To prove part 2., let ϵ and $M \geq 1$ be such that $c_n := \|\tilde{\theta}_n - \tilde{\theta}_G\| = \frac{\epsilon}{M}$ where $\theta = (\tilde{\theta}, l)$. Then, if

$$l_{n,\epsilon}^* - \epsilon\left[1 - \frac{c_n^2}{\epsilon^2}\right]^{1/2} \leq l_n \leq l_{n,\epsilon}^* + \epsilon\left[1 - \frac{c_n^2}{\epsilon^2}\right]^{1/2}$$

we have $\|\theta_n - \theta_G^{l_{n,\epsilon}^*}\| \leq \epsilon$ so that $l_n(\theta_G^{l_{n,\epsilon}^*}) \geq l_n(\theta_n)$.

B Extended skew-normal sample selection models

B.1 Prior distributions for Σ B and $\boldsymbol{\beta}_2$

When available, the conjugate prior distribution is frequently used in bayesian analysis. Under Gaussian error terms and no selection effect, the conjugate prior distribution for β_1 and Σ is the normal-inverse Wishart distribution

$$\pi(\boldsymbol{\beta}_1, \Sigma|\boldsymbol{\mu}_{\boldsymbol{\beta}_1}, \kappa, \nu, V) \propto \exp\left(-\frac{1}{2}\text{tr}(V\Sigma^{-1}) - \frac{\kappa}{2}(\boldsymbol{\beta}_1 - \boldsymbol{\mu}_{\boldsymbol{\beta}_1})'(\Sigma^{-1} \otimes c_{\boldsymbol{\beta}_1} X'X)(\boldsymbol{\beta}_1 - \boldsymbol{\mu}_{\boldsymbol{\beta}_1})\right) \times |\Sigma|^{-\frac{\nu+|\boldsymbol{\beta}_1|+2}{2}}$$

where $c_{\boldsymbol{\beta}_1}$ is a scale factor, V is a $d \times d$ positive definite matrix, κ and ν are real such that $\nu > |\boldsymbol{\beta}_1| + 3$[17]. Since the ESN distribution generalizes the Gaussian distribution, and because the presence of selection effect does not modify our prior knowledge, we choose this prior distribution for $\boldsymbol{\beta}_1$ and Σ.

Using a similar argument, a possible choice of prior distribution for the parameters of the selection equation is

$$\boldsymbol{\beta}_2 \sim \mathcal{N}_{|\boldsymbol{\beta}_2|}(\boldsymbol{\mu}_{\boldsymbol{\beta}_2}, c_{\boldsymbol{\beta}_2}(X'X)^{-1})$$

where $c_{\boldsymbol{\beta}_2}$ is a scale factor. This choice or prior distribution for (β, Σ) is particularly convenient for model selection because under Gaussian error terms and no selection effect the posterior mean of $\boldsymbol{\beta}_1$ and Σ has a closed form expression provided that $\boldsymbol{\beta}_1$ and $\boldsymbol{\beta}_2$ are a priori independent. In the numerical study (Section 4.4.2), the parameter of the prior distribution we choose are $\mu_{\boldsymbol{\beta}_1} = \mu_{\boldsymbol{\beta}_2} = 0$ and $c_{\boldsymbol{\beta}_1} = c_{\boldsymbol{\beta}_2} = 5n$ with n the number of observations and where $\boldsymbol{\beta}_1$ and $\boldsymbol{\beta}_2$ are assumed to be independent.

B.2 Determination of the marginal effects

Proposition 4.1. *Consider the univariate extended skew-normal sample selection model defined by* (4.82) *and* (4.83)*. Let*

$$\tau(a, \alpha, \lambda) = \frac{\phi(a)\Phi(\lambda + \alpha a)}{\Phi_2(a, 1, \alpha, \lambda)}, \quad \delta(a, \alpha, \lambda) = \frac{\phi(\lambda/c_0)\Phi\left(ac_0 + \frac{\alpha\lambda}{c_0}\right)}{\Phi_2(a, 1, \alpha, \lambda)}.$$

Then,

$$\mathbb{E}\left[S_i^*|S_i = 1, \mathbf{x}_i\right] = \beta_2'\mathbf{x}_i + \tau_{2i} + \frac{c_2\tilde{\alpha}_2}{c_{02}}\delta_{2i}$$
$$\mathbb{E}[Y_i^*|S_i = 1, \mathbf{x}_i] = \xi_{1i} + \mathbf{x}_i'\beta_1 + \sigma_{12}\tau_{2i} + \sigma_1 v_2 \delta_{2i}$$

[17] This last condition is not necessary but ensures that all the components of Σ has a finite variance.

where $\tau_{2i} = \tau\left(\xi_2 + \mathbf{x}_i'\beta_2, -c_2\tilde{\alpha}_2, c_2\lambda\right)$, $\delta_{2i} = \delta\left(\xi_2 + \mathbf{x}_i'\beta_2, -c_2\tilde{\alpha}_2, c_2\lambda\right)$ *and* $v_2 = \frac{\rho c_2\tilde{\alpha}_2 + c_2(1-\rho^2)\alpha_1}{c_{02}}$.

See Gerber and Pelgrin (2014) for a proof.